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CESAR AUGUSTO JARUTAI FENSTERSEIFER

**OTIMIZAÇÃO DOS PROCESSOS DE CALIBRAÇÃO E VALIDAÇÃO DO  
MODELO CROPGRO-soybean.**

Santa Maria, RS  
2016

**Cesar Augusto Jarutais Fensterseifer**

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Tese de Doutorado apresentada ao curso de Pós-Graduação em Engenharia Agrícola, Área de Concentração em Engenharia de Água e Solo, da Universidade Federal de Santa Maria (UFSM,RS), como requisito parcial para obtenção do grau de **Doutor em Engenharia Agrícola.**

Orientador: Prof. Nereu Augusto Streck

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Santa Maria,  
06 de Dezembro de 2016..

## DEDICATÓRIA

*Dedico ao meu pai Jorge Luis Fensterseifer e à minha avó Ermínia Sausen Fensterseifer, por não medirem esforços, dedicação e apoio, em minha formação moral e profissional durante toda a minha jornada.*

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A boa educação de um homem,  
é a sua melhor garantia contra a  
má educação dos outros.  
(Lord Chesterfield).

## RESUMO

### OTIMIZAÇÃO DOS PROCESSOS DE CALIBRAÇÃO E VALIDAÇÃO DO MODELO CROPGRO-soybean.

AUTOR: CESAR AUGUSTO FENSTERSEIFER  
ORIENTADOR: NEREU AUGUSTO STRECK

Modelos agrícolas são ferramentas importantes para aprimorar técnicas de manejo e consequentemente a eficiência dos sistemas agrícolas. Esse acréscimo na eficiência são úteis para atender a crescente demanda de alimentos e combustíveis, sem avançar a fronteira agrícola. A calibração e validação de um modelo agrícola, historicamente considerou conjuntos de dados que variam de poucos a muitos experimentos. Poucos experimentos podem aumentar as incertezas e muitos experimentos tem alto custo financeiro e demanda de tempo. Pelo método de partição em dois grupos, o conjunto de experimentos é dividido em duas partes, uma para calibrar e a outra validar o modelo. Se apenas um conjunto pequeno de experimentos está disponível, dividi-los pode prejudicar o desempenho do modelo. Assim, métodos que otimizem esses processos, diminuindo o tempo e o custo de experimentos necessários para a calibração e validação, são sempre bem vindos. O objetivo do primeiro capítulo desta tese, foi comparar o método tradicionalmente utilizado na calibração e validação de modelos com um método mais robusto (cross-validation). Ambos os métodos foram aplicados para estimar os coeficientes genéticos na calibração e validação do modelo CROPGRO-soybean, utilizando múltiplos experimentos. Um conjunto com os 3 experimentos mais detalhados foram utilizados para calibração utilizando o método de partição em dois grupos. Já o método cross-validation, foi aplicado utilizando 21 experimentos. A cultivar NA5909 RG foi selecionada por ser uma das mais cultivadas no sul do Brasil nos últimos 5 anos, conduzida em experimentos distribuídos em oito locais do Estado do Rio Grande do Sul durante as safras de 2010/2011 até 2013/2014. O método cross-validation reduziu os RMSEs encontrados no método tradicionalmente utilizado de 2.6, 4.6, 4.8, 7.3, 10.2, 677 e 551 para 1.1, 4.1, 4.1, 6.2, 6.3, 347 e 447 para emergência, R1, R3, R5, R7 (em dias), grãos.m<sup>-2</sup> e kg.ha<sup>-1</sup>, respectivamente. Foi observado estabilidade na maioria das estimativas de coeficientes genéticos, o que sugere a possibilidade de utilizar um menor número de experimentos no processo. Considerando a ampla faixa de condições ambientais, o modelo apresentou desempenho satisfatório na previsão fenológica, de biomassa e produtividade. Para otimizar os processos de calibração e validação, indica-se que o método cross-validation seja utilizado sempre que possível. No segundo capítulo, o principal objetivo foi avaliar o desempenho do uso de diferentes números de experimentos, e estimar o número mínimo necessário para garantir desempenho satisfatório do modelo CROPGRO-soybean. Esse estudo também utilizou 21 experimentos, com a cultivar BMX Potência RR. Os experimentos foram organizados em quatro grupos: Grupo 1 (semeaduras individuais), grupo 2 (ano agrícola por local), grupo 3 (local experimental) e grupo 4 (todos os experimentos juntos). Conforme o número de experimentos aumentou, a variabilidade dos coeficientes e os erros relativos (RRMSE) diminuíram. O primeiro grupo apresentou os maiores erros relativos, com até 28.4, 48 e 36% de erros nas simulações de R1, IAF e produtividade, respectivamente. O maior decréscimo nos erros relativos, ocorreu quando avançamos do grupo 1 para o grupo 2. Em alguns casos os erros foram reduzidos em mais que duas vezes. Assim, considerando o elevado custo financeiro e a demanda de tempo que os grupos 3 e 4 apresentam, recomenda-se a escolha de pelo menos o grupo 2, com 3 experimentos no mesmo ano agrícola. Essa estratégia vai permitir um melhor entendimento sobre o desempenho da cultivar, além de calibrar e validar o modelo CROPGRO-soybean, evitando os altos custos de vários experimentos, garantindo o desempenho satisfatório do modelo.

Palavras-chave: CROPGRO-soybean. Modelo agrícola. Cross-validation.

## ABSTRACT

### OPTIMIZATION OF THE CROPGRO-soybean MODEL CALIBRATION AND VALIDATION PROCESSES

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Crop models are important tools to improve the management and yield of agricultural systems. These improvements are helpful to meet the growing food and fuel demand without increase the crop areas. The conventional approach for calibrating/validating a crop model considers few to many experiments. However, few experiments could lead to higher uncertainties and a large number of experiments is too expensive. Traditionally, the classical procedure use to share an experimental dataset one part to calibrate and the other to validate the model. However, if only few experiments are available, split it could increase the uncertainties on simulation performance. On the other hand, to calibrate/validate the model using several experiments is too expensive and time consuming. Methods that can optimize these procedures, decreasing the processing time and costs, with a reliable performance are always welcome. The first chapter of this study was conducted to evaluate and compare a statistically robust method with the classical calibration/validation procedure. These two procedure, were applied to estimate the genetic coefficients of the CROPGRO-soybean model, using multiple experiments. The cross-validation leave-one-out method, was applied to 21 experiments, using the NA 5909 RG variety, across a southern state of Brazil. The cross-validation reduced the classical calibration/validation procedure average RMSE from 2.6, 4.6, 4.8, 7.3, 10.2, 677 and 551 to 1.1, 4.1, 4.1, 6.2, 6.3, 347 and 447 for emergence, R1, R3, R5, R7 (days), grains.m<sup>-2</sup> and kg.ha<sup>-1</sup>, respectively. There was stability in the estimated ecotype and genetic coefficient among the 21 experiments. Considering the wide range of environment conditions, the CROPGRO-soybean model provided robust predictions of phenology, biomass and grain yield. Finally, to improve the calibration/validation procedure performance, the cross-validation method should be used whenever possible. For the second chapter of this study, the main objectives were to evaluate the calibration/validation uncertainties using different numbers of experiments and to find out the minimum number of experiments required for a reliable CROPGRO-Soybean simulation. This study also used 21 field experiments (BMX Potencia RR variety) sown in eight different locations of Southern Brazil between 2010 and 2014. The experiments were grouped in four classes (Individual sowings, season/year per location, experimental sites, and all data together). As the grouping level increase, the developmental stages RRMSE (%), decreased from 22.2% to 7.8% from individual sowings to all data together, respectively. The use of only one individual sowings experiment could lead to a RRMSE of 28.4, 48, and 36% for R1, LAI and yield, respectively. However, the largest decrease occurred from the individual sowings to the season/year per location. Then, is recommended, use at least the season/year per location (early, recommended and late sowing dates) class. It will allow understand the behavior of the variety, avoiding the high costs of several experiments and keeping a reliable performance of the model.

Key words: CROPGRO-soybean, crop model, cross-validation.

## SUMÁRIO



<b>1</b>	<b>INTRODUÇÃO.....</b>	<b>11</b>
<b>2</b>	<b>REVISÃO DE LITERATURA .....</b>	<b>12</b>
2.1	A cultura da soja .....	12
2.2	Modelos de simulação do crescimento, desenvolvimento e produtividade das culturas .....	14
2.3	Modelo CROPGRO .....	16
<b>3</b>	<b>OBJETIVO GERAL .....</b>	<b>20</b>
<b>4</b>	<b>OBJETIVOS ESPECÍFICOS .....</b>	<b>20</b>
<b>5</b>	<b>ARTIGO 1.....</b>	<b>21</b>
	Abstract .....	22
	1. INTRODUCTION.....	23
	2. DATA AND METHODS .....	25
	3. RESULTS AND DISCUSSION .....	35
	4. CONCLUSIONS .....	44
	5. ACKNOWLEDGEMENTS .....	45
	<u>6. REFERENCES.....</u>	45
<b>6</b>	<b>ARTIGO 2.....</b>	<b>48</b>
	Abstract .....	49
	1. INTRODUCTION .....	49
	2. DATA AND METHODS .....	51
	3. RESULTS .....	58
	4. DISCUSSION.....	62
	5. CONCLUSIONS .....	63
	6. ACKNOWLEDGEMENTS .....	64
	7. REFERENCES .....	64
<b>7</b>	<b>DISCUSSÃO .....</b>	<b>68</b>
<b>8</b>	<b>CONCLUSÃO .....</b>	<b>71</b>
<b>9</b>	<b>REFERÊNCIAS.....</b>	<b>72</b>
<b>10</b>	<b>APÊNDICE.....</b>	<b>73</b>



## 1 INTRODUÇÃO

O aumento na demanda por alimentos e fontes alternativas de energia no mundo, exerce crescente pressão nos recursos naturais, visando o aumento da produtividade das culturas, sem avançar as fronteiras agrícolas. Importante fonte de proteína para alimentação animal e humana, a cultura da soja (*Glycine max* (L.) Merrill) é a oleaginosa mais produzida no mundo. Entre inúmeros subprodutos, destaca-se como principal fonte de biodiesel (quase 80%) para suprir a demanda energética do Brasil (ABIOVE, 2016). A produção mundial de soja quase triplicou nos últimos 20 anos, passando de 127 para em torno de 330 milhões de toneladas (1995 – 2016/17, USDA). Estados Unidos, Brasil, Argentina e China são os maiores produtores mundiais (somam em torno de 85% da produção global) de soja e estima-se que produzirão 114, 101 e 57 milhões de toneladas na safra 2016/17, respectivamente.

A crescente demanda por cultivares de soja mais resistentes e produtivas, faz com que as empresas acelerem o lançamento de novas cultivares, e conseqüentemente, diminuam o período e a abrangência dos testes. Essas restrições nos experimentos e avaliações, aumentam as incertezas sobre o real desempenho da cultivar em diferentes regiões e/ou sob diferentes manejos. O conhecimento mais detalhado das interações genótipo x ambiente x manejo, aumentaria a eficiência do planejamento agrícola e o desempenho das cultivares nas lavouras.

Propostos há mais de 50 anos (modelo GOSSYM) (EL-Sharkawy, 2011)), modelos agrícolas, são ferramentas que sintetizam o conhecimento de anos de pesquisa sobre os processos físicos, químicos, biológicos e suas interações (Ma et al., 2000). Entre os vários modelos disponíveis para soja, destaca-se o modelo CROPGRO-soybean (Boote et al., 1998), um modelo mecanístico, com base fisiológica, que simula o crescimento, desenvolvimento e produtividade de soja em função das condições ambientais, manejo e características da cultivar. O modelo faz parte do Sistema de Suporte à Decisão e Transferência de Agrotecnologia (DSSAT), capaz de simular mais de 28 culturas. Após devidamente calibrados, os modelos são alternativas de baixo custo, capazes de replicar experimentos pontuais e simular ilimitadamente as interações genótipo x ambiente x manejo de uma cultivar.

Tradicionalmente, ao calibrar e validar um modelo, um conjunto de experimentos é dividido em duas partes, uma para a calibração e outra para a validação (Garrison et al., 1999). Ao utilizar um número limitado de experimentos, dividi-los em duas partes pode afetar negativamente o desempenho da calibração e validação (Thorp et al., 2007). Além disso, quanto maior o número de experimentos, melhor é o desempenho das simulações de produtividade do modelo (Thorp et al., 2007). Os altos custos de tempo e financeiro que demanda a condução múltiplos experimentos, estão entre as principais dificuldades enfrentadas na expansão da utilização de ferramentas como modelos agrícolas.

Assim, alternativas capazes de otimizar e reduzir o número de experimentos necessários para calibrar e validar o modelo agrícola, sem comprometer o desempenho durante a validação, incentivaria a pesquisa e utilização de ferramentas que simulam as culturas. Quanto mais próxima dos tomadores de decisões essas ferramentas estiverem, maior o entendimento sobre o comportamento das cultivares e conseqüentemente, a eficiência do planejamento agrícola. Os objetivos deste trabalho são: 1) Testar e avaliar o desempenho de dois métodos de calibração e validação do modelo CROPGRO-soybean e 2) quantificar as incertezas causadas pelo uso de diferentes números de experimentos na calibração e validação do modelo CROPGRO-soybean.

## **2 REVISÃO DE LITERATURA**

### **2.1 A CULTURA DA SOJA**

A cultura da Soja (*Glycine max* (L.) Merrill) teve sua origem no século XI a.C. no norte da China, a partir do cruzamento de duas espécies de soja selvagens, que foram melhoradas e domesticadas (Dall'agnol et al., 2007). No Brasil, as primeiras referências da cultura ocorreram no Estado da Bahia (utilizada como forrageira) em 1882. O cultivo comercial surgiu a partir de 1914, na região noroeste do Estado do Rio grande do Sul (Santa Rosa), onde as condições climáticas se assemelham às condições de origem e as que eram cultivadas no sul dos Estados Unidos (Zanon et. al., 2015). Atualmente os principais produtores mundiais são os Estados Unidos,

Brasil, Argentina e China, responsáveis por mais de 87% da produção mundial (USDA – Departamento de Agricultura dos Estados Unidos, 2017).

Na safra 2015/2016, a área cultivada com soja no mundo foi de 119,732 milhões de hectares com uma produção de 313.2 milhões de toneladas (USDA, 2016). O Brasil é o segundo maior produtor mundial de soja. Na safra 2016/2017 serão cultivados em torno de 34 milhões de hectares, totalizando uma produção estimada entre 102 e 104 milhões de toneladas (CONAB, 2016). Na safra (2012/2013) o Brasil alcançou pela primeira vez na história o título de maior produtor mundial de soja, após os Estados Unidos registrarem a maior estiagem no país desde 1956 (USDA, 2013).

No Brasil, a soja é a cultura agrícola que mais cresceu nas últimas três décadas e atualmente corresponde a quase 60% da área plantada em grãos do país (CONAB, 2016) (Figura 1).

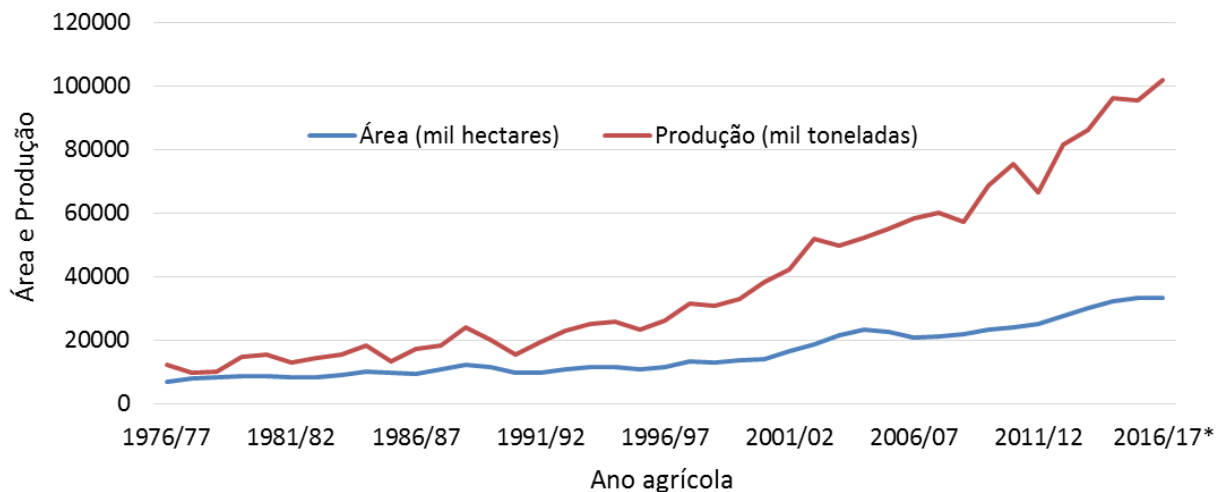


Figura 1: Evolução histórica da área semeada e produção de soja no Brasil (\* produção e Área estimadas).

Com aproximadamente 38% de proteínas, 19% de lipídios, 23% de carboidratos e 17% de fibra alimentar na composição nutricional, é crescente o número de subprodutos derivados a partir do grão de soja. Essa grande quantidade de subprodutos que se derivam da soja, faz com que a cultura apresente alto valor econômico, tanto em nível nacional, quanto internacional (Silva et al., 2006). Os derivados abastecem demandas como a alimentação humana, nutrição animal, usos industriais, biocombustíveis, além de ser a matéria prima mais importante do mundo para a produção de óleo comestível (Borrmann, 2009).

A soja é a principal oleaginosa utilizada para suprir o avanço do percentual de biocombustível estipuladas pelo PNPB (Programa Nacional de Produção e Uso de Biodiesel), responsável por aproximadamente 80% da produção de biodiesel (PNPB, 2013). O país apresentou um expressivo salto na produção de grãos de soja nos últimos anos, de aproximadamente 75 milhões para 103 milhões de toneladas nas safras de 2010/2011 e 2016/17, respectivamente (CONAB, 2016), ou seja, um aumento em torno de 37% na produção. Já nas exportações de soja no mesmo período citado acima, apresentaram um aumento de aproximadamente de 72% (CONAB, 2016).

A Região Sul do Brasil está em segundo lugar em área cultivada e produção de soja (19,209 milhões de ha), ficando atrás apenas da Região Centro-Oeste, onde o Estado do Mato Grosso é o maior produtor, seguido pelo Paraná e pelo Rio Grande do Sul (CONAB, 2016) (Figura 2). Desses três Estados, o RS é o que apresenta a menor média de produtividade, parcialmente explicada por recorrentes estiagens em estágios críticos da cultura.

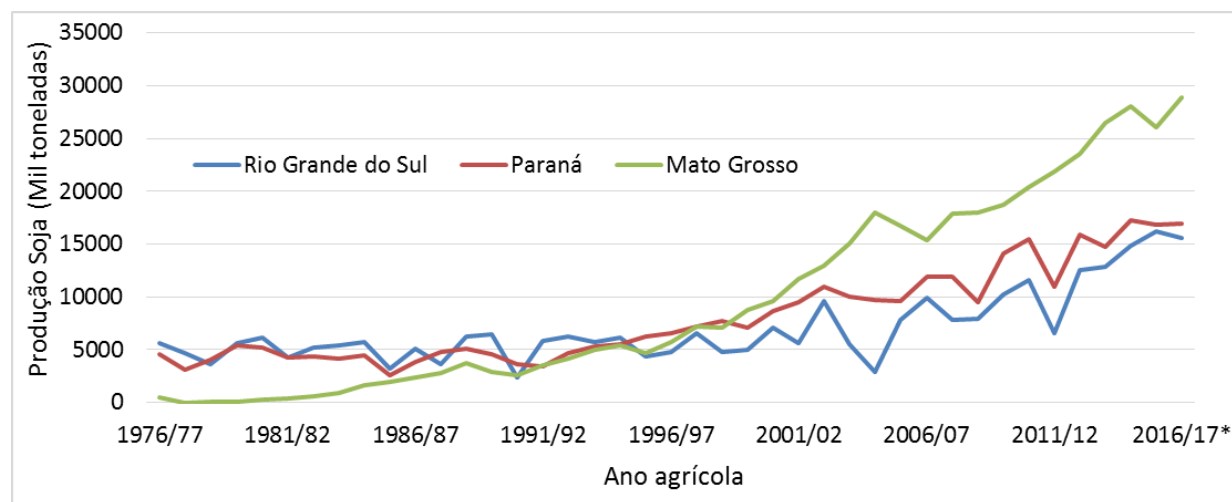


Figura 2: Evolução da produção de soja nos principais produtores estaduais do Brasil.

## 2.2 MODELOS DE SIMULAÇÃO DO CRESCIMENTO, DESENVOLVIMENTO E PRODUTIVIDADE DAS CULTURAS

Existem inúmeros modelos de simulação de culturas na literatura que possibilitam a estimativa de produtividade de grãos. Modelos matemáticos são ferramentas úteis para caracterizar o crescimento e o desenvolvimento das culturas agrícolas (Streck et al., 2008a). Entre os diversos tipos de modelos, os mais simples são os empíricos, que estabelecem relações simplificadas entre algumas (uma a três) variáveis (meteorológicas, por exemplo) e a produtividade de uma determinada cultura. São geralmente compostos por equações diretas obtidas pelas curvas de correlação entre determinadas variáveis. Entre inúmeros exemplos, o modelo empírico proposto por Thenkabail et al., (1994) (equação 1) que estima o índice de área foliar (IAF) da cultura da soja baseado no índice de vegetação com diferença normalizada (NDVI).

$$\text{Equação 1.} \quad \text{IAF} = 0,511e^{5,167 \cdot \text{NDVI}}$$

Entre os modelos mais complexos, destacam-se os mecanísticos, que são capazes de simular todos os processos e interações envolvidos na produção de matéria seca durante o crescimento, desenvolvimento e produtividade das culturas (Dourado-Neto et al., 1998). Apesar da maioria dos modelos mecanísticos necessitar de um maior número de variáveis iniciais, de modo geral, apresentam desempenho superior se comparados a outros tipos de modelos.

Partindo do princípio de que as plantas respondem ao meio, a maioria dos modelos de simulação de culturas utilizam as temperaturas cardinais das culturas para calcular a soma térmica necessária para estimar a taxa de crescimento. Temperaturas cardinais são compostas pela temperatura base ( $T_b$ ), temperatura ótima 1 ( $T_{Opt1}$ ), temperatura ótima 2 ( $T_{Opt2}$ ) e temperatura máxima ( $T_{max}$ ). A temperatura base, é o valor limite em que abaixo o crescimento é nulo ou irrelevante. As temperaturas ótimas são o intervalo no qual a taxa de crescimento é máximo para a cultura. Já a temperatura máxima, é o valor no qual a taxa de crescimento é nula.

Modelos agrícolas são ferramentas poderosas, que sintetizaram todo o conhecimento obtido durante décadas de experimentos conduzidos no campo, em ambientes controlados e laboratórios. Isso os torna capazes de simular os principais processos das plantas, como a fotossíntese, evapotranspiração, distribuição de água no solo, dinâmica de nutrientes na planta e no solo, transferências de energia e o crescimento da cultura dia após dia. Esse elevado nível de detalhamento, permite a avaliação do desempenho de cultivares em diferentes regiões, solos, condições climáticas e datas de semeadura (Soler, Sentelhas & Hoogenboom, 2009). Essas

avaliações podem minimizar as incertezas sobre as interações genética x ambiente x manejo, impactos do clima, e aprimorar a irrigação, fertilização e o melhoramento genético (Thorp et al., 2014).

No caso da soja, diversos modelos simulam mudanças físicas, químicas e processos biológicos na planta em função da disponibilidade dos elementos meteorológicos, tipos de solo e manejo da cultura (Vera-Diaz, 2008). Essa caracterização é importante, pois permite projetar a data de ocorrência de alguns estádios de desenvolvimento, bem como a previsão de duração das fases vegetativa e reprodutiva e o período de sobreposição das mesmas, o que é importante para a realização do manejo e também para escolha de cultivares com maior estabilidade de produção (Marchezan, 1982; Rodrigues et al., 2001). Alguns dos modelos de simulação da cultura da soja incluem: o modelo SOYBEAN (Sinclair, 1986), o modelo GLYCIM (Acock; Trent, 1991), o modelo SOYCROS (Penning de Vries et al., 1992), o modelo CROPGRO–soybean (Boote et al., 1998), e os modelos SOYDEV e SOYSIM (Setiyono et al., 2007; 2010).

O modelo CROPGRO faz parte da plataforma Decision Support System for Agrotechnology Transfer (DSSAT) (Hoogenboom et al., 2004), juntamente com outros modelos que somados, simulam 28 culturas agrícolas. Atualmente a plataforma DSSAT está na versão 4.6 (Hoogenboom, 2012). Para executar as simulações no modelo CROPGRO-soybean, é necessário supri-lo com dados meteorológicos diários de temperaturas máximas e mínimas, radiação solar e precipitação pluviométrica. Para aumentar a precisão das simulações, são necessárias informações detalhadas sobre o experimento e as condições ambientais.

### 2.3 MODELO CROPGRO

O modelo CROPGRO foi construído baseado nos modelos SOYGRO, PNUTGRO e BEANGRO, para simular legumes e, posteriormente adaptado para outras culturas como Amendoim, Feijão, Grão de Bico, Feijão de Corda, Vagem, Tomate, Feijão da Flórida, Braquiária, Grama Bahia, Algodão, Repolho, Pimentão, Mandioca, Batata, Cana de açúcar, Tomate e Girassol (DSSAT version 4.6). O modelo CROPGRO calcula a fotossíntese do dossel em intervalos de tempo por hora, utilizando parâmetros de fotossíntese a nível de folha, com cálculos da



interceptação de luz na entrelinha e na cobertura. O CROPGRO é um modelo baseado em processos que considera o balanço de Carbono na cultura, o balanço de Nitrogênio no solo e o balanço hídrico (Ines et al. 2001).

O modelo CROPGRO-soybean, foi desenvolvido para simular o crescimento, desenvolvimento e a produtividade de soja em função das características específicas da cultivar (duração dos estágios fenológicos, estrutura, tamanho e formato de folhas, ...), condições do solo, do clima e do manejo (cultivar, espaçamento, densidade, data de semeadura, fertilização e irrigação) (Jones et al. 2003). Esses processos simulam a fotossíntese, respiração, acúmulo e partição de biomassa, extração de água do solo, evapotranspiração e sequestro de nutrientes do solo. Para simular o crescimento, desenvolvimento e produtividade de forma mais precisa, o modelo CROPGRO-soybean deve ser calibrado, utilizando dados observados em experimentos.

Para a calibração dos estádios fenológicos de uma cultivar, são utilizados dados observados em experimentos de campo. A data de cada estágio fenológico é estimada quando mais de 50% das plantas monitoradas, atingem determinado estágio. Esses estádios fenológicos foram estimados de acordo com a escala de Fehr & Caviness (1977), e posteriormente, foram utilizados apenas os estádios que o modelo CROPGRO-soybean necessita (Emergência, R1, R3, R5 e R7). O estágio R1 é o aparecimento da primeira flor na haste principal, considerado o início do florescimento. O R3 e R5 são o início da formação do legume e início do enchimento de grãos, respectivamente, e são determinados nos últimos 4 nós da haste principal. Finalmente o estágio R7, que é o início da maturação fisiológica da planta, quando um dos legumes se encontra na cor amarela. Esses dados são então transformados para dias após a emergência (DAS), valores obtidos como resultados nas simulações.

Assim, a cada simulação realizada, o valor de DAS simulado é comparado com o observado, e se necessário, os coeficientes são modificados novamente, até que os valores apresentem o menor erro médio quadrático possível.

Tabela 1: Descrição dos coeficientes genéticos que foram modificados durante a calibração de novos cultivares.

Coeficiente	Descrição
Coeficientes de desenvolvimento	
CSDL	Também chamada de CSDVAR, comprimento crítico do dia, acima do qual o processo de desenvolvimento reprodutivo não é afetado (horas);

PPSEN	Inclinação da resposta relativa do desenvolvimento para fotoperíodo com o tempo ( $1.\text{hora}^{-1}$ );
EM-FL	Período entre a emergência da planta e o aparecimento da primeira flor (R1) (dias fototermais);
FL-SH	Período entre o aparecimento da primeira flor e a primeira legume (R3) (dias fototermais);
FL-SD	Período entre o aparecimento da primeira flor e o início da formação do grão (R5) (dias fototermais);
SD-PM	Período entre o início da formação do grão e a maturidade fisiológica (R7) (dias fototermais);
FL-LF	Período entre o aparecimento da primeira flor (R1) e final da expansão foliar; Coeficientes de crescimento
LFMAX	Taxa máxima de fotossíntese da folha a uma taxa ótima de temperatura $30^{\circ}\text{C}$ ( $\text{mg CO}_2.\text{m}^{-2}.\text{s}^{-1}$ );
SLVAR	Área foliar específica sob condições normais de crescimento;
SIZLF	Tamanho máximo da folha completamente expandida ( $\text{cm}^2$ );
XFRT	Máxima fração do crescimento diário que é particionada para a semente mais a vagem;
WTPSD	Peso máximo de um grão (g);
SFDUR	Tempo necessário para que o enchimento de grãos do último legume esteja completo sob condições de crescimento ótimas (dias fototermais);
PODUR	Duração do enchimento de grão na cavidade do legume em condições normais de crescimento (dias fototermais);

De acordo com Dallacort et al., (2005), o modelo CROPGRO-soybean apresentou alta sensibilidade à variação dos coeficientes genéticos dos cultivares estudados. A distribuição da precipitação pluviométrica foi um dos fatores que mais influenciou no índice de área foliar e na produtividade, ou seja, o modelo penaliza o crescimento, desenvolvimento e produtividade severamente em condições de déficit hídrico.

Para padronizar e fazer com que todos os modelos da plataforma DSSAT utilizem o mesmo processo de balanço hídrico do solo, as simulações são realizadas pelo módulo SWAP (solo-água-planta-atmosfera) separado do restante do modelo. Para simular o balanço hídrico no solo, o modelo necessita de informações físicas detalhadas de todas as camadas individualmente. Em cada camada, a espessura, ponto de murcha, capacidade de campo, saturação, fator de crescimento das raízes, condutividade hidráulica saturada, densidade, textura, acidez do solo e capacidade de troca de cátions (CTC), precisam ser informados. Informações sobre o albedo, limite de evaporação diária, taxa de drenagem diária, curva de escoamento superficial e fertilidade do solo também devem ser informados.

A infiltração é calculada subtraindo o escoamento superficial do volume total de chuva a cada dia. O método SCS (Soil Conservations Service, 1972) é utilizado para particionar o volume total, em infiltração e escoamento superficial. O método SCS, leva em conta a textura, declividade e forma da sementeira (plantio direto ou convencional), para estimar o escoamento superficial pela curva número. O método foi melhorado (Williams et. al. 1984), para levar em conta todas as camadas do solo e os respectivos conteúdos de água no momento em que a precipitação pluviométrica ocorre.

Para simular o balanço hídrico e fluxo descendente de água entre as camadas do solo, é utilizado o método cascata (RITCHIE, 1998), em que a drenagem da água só ocorre a partir do momento que o volume de água é superior a capacidade de campo. O fluxo de água através de uma camada é estimado de acordo com os parâmetros físicos, e posteriormente comparada pela condutividade hidráulica saturada da respectiva camada. Se a taxa de infiltração estimada for maior que a condutividade hidráulica da camada, mantém-se a condutividade hidráulica e o restante é armazenado na camada superior. Esse processo garante maior precisão ao simular solos com baixa capacidade de drenagem. O movimento de fluxo ascendente é simulado a partir de uma equação da difusividade de água no solo, que leva em conta as diferenças volumétricas do conteúdo de água das camadas adjacentes, parametrizada para solos de diferentes texturas (Jones et. al, 2003).

Timsina et. al., 2007, testaram o desempenho do modelo CROPGRO-soybean ao simular os danos causados pela perda de folhas e vagens causada por insetos durante diferentes estádios da cultura. Em geral, a previsão de perda de vagens foi precisa, porém, é necessária a avaliação da simulação do aparecimento de vagens tardias, após a defoliação. Concluíram que o modelo apresentou capacidade adequada para ser usado como ferramenta para quantificar os danos causados pela queda de vagens e folhas em diferentes períodos e intensidades na cultura da soja.

Alagarswamy et. al., 2006, avaliaram o desempenho do modelo CROPGRO-soybean na simulação das respostas fotossintéticas a diferentes níveis de dióxido de carbono. As simulações representaram de forma correta (valores da literatura) os efeitos do aumento na concentração de dióxido de carbono na atmosfera. Os resultados obtidos no índice de concordância de Willmott variaram entre 0,86 a 0,99, o que dá credibilidade ao uso do modelo CROPGRO-soybean.

### **3 OBJETIVO GERAL**

Otimizar o método e o número de experimentos necessários nos processos de calibração e validação, sem prejudicar o desempenho do modelo CROPGRO-soybean.

### **4 OBJETIVOS ESPECÍFICOS**

1 – Avaliar o desempenho do método cross-validation Leave-One-Out e o método de partição em dois grupos (tradicionalmente utilizado) aplicados na calibração e validação do modelo CROPGRO-soybean;

2 – Quantificar as incertezas na utilização de diferentes números de experimentos na calibração e validação do modelo CROPGRO-soybean, buscando um número ótimo de experimentos.

**5 ARTIGO 1**

**CALIBRATING ECOTYPE AND GENETIC COEFFICIENTS FOR MODELING  
SOYBEAN USING CROSS-VALIDATION ON MULTIPLE EXPERIMENTAL FIELDS**

(Artigo submetido para publicação na revista Engineering in Agriculture, Environment and  
Food)

## Calibrating ecotype and genetic coefficients for modeling soybean using cross-validation on multiple experimental fields

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### Abstract

Crop models are important tools to improve the management and yield of agricultural systems. These improvements are helpful to meet the growing food and fuel demand without increase crop areas. Performance improvements, such as decrease calibration and validation processing time and increase accuracy are always needed. This study was conducted to compare a statistically robust method with the traditionally used two-group partition method (by Thorp et al., 2007), to calibrate/validate and estimate ecotype and genetic coefficients of CROPGRO-soybean model using multiple experiments. Cross-validation method was applied to 21 experiments across a southern state of Brazil. The cross-validation reduced the classical calibration/validation procedure average RMSE from 2.6, 4.6, 4.8, 7.3, 10.2, 677 and 551 to 1.1, 4.1, 4.1, 6.2, 6.3, 347 and 447 for emergence, R1, R3, R5, R7 (days), grains.m<sup>-2</sup> and kg.ha<sup>-1</sup>, respectively. There was stability in the estimated ecotype and genetic coefficient among the 21 experiments. Considering the wide range of environment conditions, the CROPGRO-soybean model provided robust predictions of phenology, biomass and grain yield. Finally, to improve the coefficients estimation and simulation performance, the cross-validation method should be used whenever possible.

**Key words:** soybean, genetic coefficients, uncertainty, cross-validation, crop models, CROPGRO-soybean

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## 1. INTRODUCTION

Soybean (*Glycine max* (L.) Merrill) is the most produced oilseed crop worldwide (FAO, 2013). After the USA, Brazil is the second higher soybean producer, comprising approximately 31% of the total world soybean production (nearly 283 Million tons) in 2013/14 (USDA, 2015). The country has seen a significant increase in soybean cropping area during the last three decades currently covering 56% of the total summer cropped area (CONAB, 2015). Besides its use in food and feed, it has been increasingly used to produce biofuel and it is the source of more than 70% of the total biofuel used to supply the goals of the National Program for Production and Use of Biodiesel (PNPB), around 4 billion of liters in 2015.

Rio Grande do Sul (RS) is the largest biodiesel-producing and the third largest soybean-producing State in Brazil, and this state is responsible for 28.3% (APROBIO, 2015) and 15.6% (CONAB, 2015) of the Brazilian national production of these commodities. However, RS is also the State with the highest variability in soybean yields, mainly due to severe droughts in critical developmental stages (flowering and grain filling), as almost all of soybean production in RS is rainfed.

Crop models represent important and widely used tools for different purposes. After proper calibration, crop models may be used to predict the yields of specific genotypes and evaluate management options for them under different growing conditions. Crop models have been used for more than 40 years for different crops worldwide, including soybeans (Sinclair, 1986; Boote et al., 1997; Setiyono et al., 2010). Of all the available soybean crop models, one of the most used is the CSM-CROPGRO-soybean (Boote et al., 1998) model, as part of the Decision Support System for Agrotechnology Transfer (DSSAT; Jones et al., 2003).

In order to increase the reliability and usefulness of crop models, proper calibration is necessary. Genetic coefficients (coefficients that are specific for cultivars or varieties) are one of the major inputs (Irmak et al., 2000) used to test a model's robustness for simulating crop growth, development and yield in a range of soybean growing regions (Mavromatis et al., 2002). However, genetic coefficients may be affected by varying growing conditions, as demonstrated for soybean cultivars grown in Georgia and North Carolina States using the CROPGRO-Soybean model (Mavromatis et al., 2001). Among possible reasons that genetic coefficients are not stable in different growing conditions, temperature functions that drive development and growth processes may be incorrect (Mavromatis et al., 2001). Furthermore, new soybean cultivars are released annually, and the implications of these new releases every year is that genetic coefficients in crop simulation models are quickly outdated. Here in Brasil, about 150 new soybean varieties are launched and registered every annually.

The calibration of the genetic coefficients are usually time-consuming and expensive, as there is a need to conduct field experiments in several sowing dates and in different locations. As a consequence of varying genetic coefficients and the need for updating genetic coefficients for new cultivars, model performance can be greatly affected. Irmak et al. (2002) evaluated six genotypes of soybean, representing the maturity group VII, over five different locations and years (1987-1996) in Georgia (USA), resulting in forty place-year combinations. They found that the uncertainties associated with varying the genotypic coefficient amounted to 21% of the average yield of six genotypes (a root-mean-square error of prediction (RMSEP) of 448 kg ha<sup>-1</sup>). Part of such uncertainties may be associated with the calibration procedure. The classical approach in which the dataset is divided into two groups, one for calibration and the other for validation (Garrison et al., 1999; Zhao et al., 2000; Bakhsh et al., 2001) may not take into account all the



variability in the data and thereby impair the ability of models to simulate the observed variability over time and space.

Considering the above uncertainties, two questions may arise: Is it possible to decrease the uncertainties in simulated yields by improving current methods of estimating the genetic coefficients? Is it possible to develop a multiple-site calibration method for a crop model? This study was carried out to help answer these questions. The objective of this study was to apply and compare an statistically robust method to calibrate/validate genetic coefficients against the traditional calibration/validation method using multiple experiments.

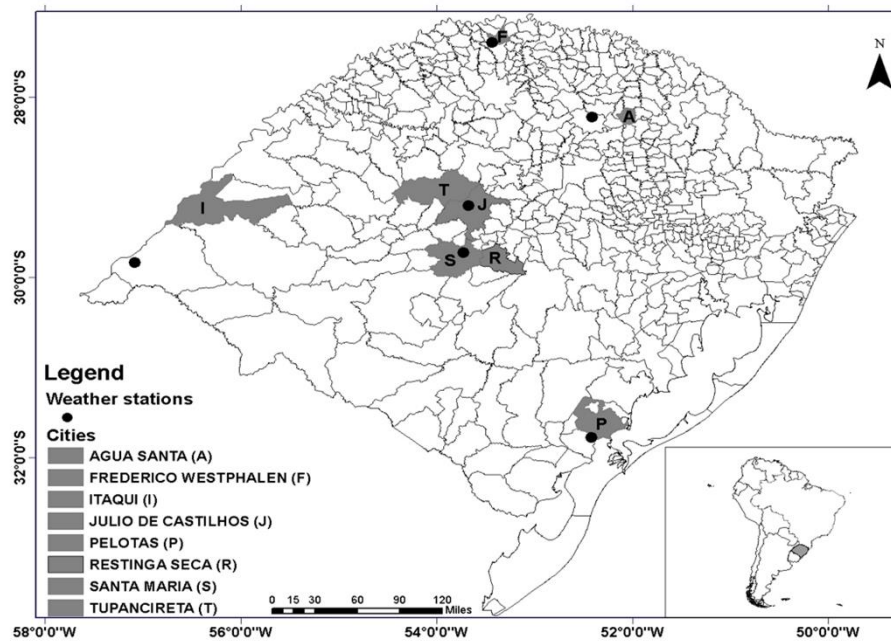
## **2. DATA AND METHODS**

### **2.1 Field experiment data**

The experiments were located in eight different cities across of the RS State, and comprised experiments conducted in government institutions (universities and state foundations) and experiments conducted in commercial farmers. The governmental institutions were the State Foundation of Agricultural Research - Fepagro (located in Julio de Castilhos), the Federal University of Pampa (in Itaqui city), the Federal University of Pelotas (in Pelotas) and the Federal University of Santa Maria (in Santa Maria and Frederico Westphalen). The farms were located in the cities of Água Santa, Tupanciretã and Restinga Seca, and the on-farm experiments were conducted under the same soil and crop management used by each farmer.

These eight sites were selected because they represent different regions where soybean is grown, covering most of the environment conditions of the state. The cities of Itaqui and Pelotas, are regions where soybean is grown in lowlands, as a rotation crop with rice and represents the

west and South region of the State, respectively. Água Santa and Frederico Westphalen represents important high lands soybean regions with deep soils, located in the north region of the State. Tupanciretã and Júlio de Castilhos, rank as the first and the third larger soybean grown area in the state. The cities of Santa Maria and Restinga Seca are mostly counties with small farming systems, both locates under the central region of the State (Figure 1).



**Figure 1:** Map of the State of Rio grande do Sul (RS), Brazil. Grey polygons indicates the cities under the field experiments were conducted. Solid circles indicates the weather stations used in simulations (the closest weather station with available data).

The field experiments were conducted and managed following recommended practices for soybean in southern Brazil. Briefly, seeds were inoculated, nutrients were applied according to soil tests for maximum yields. Weeds, pathogens and insect pests were controlled to keep the experiments free of biotic stresses. A total of 21 experiments were conducted (Table 1) during four growing seasons (from 2010/2011 to 2013/2014). The experimental design was a complete randomized block, with four replications. The frequency of field measurements and visual

observations (phenological observations, node number, the planting dates and the information about the irrigation regimes) used in each experiment are shown in Table 1.

**Table 1:** Experiments with soybean conducted during four growing seasons (2010/2011, 2011/2012, 2012/2013 e 2013/2014) at eight locations in the state of Rio Grande do Sul, Brazil.

Experiment	Crop season	Location	Sowing date	Irrigation (mm)	Measurement frequency <sup>1</sup>
1	2010/11	Santa Maria	12/10/2010	NM	Daily
2	2010/11	Santa Maria	01/08/2011	NM	Daily
3	2011/12	Santa Maria	09/24/2011	193	Daily
4	2011/12	Santa Maria	11/19/2011	130	Daily
5	2011/12	Santa Maria	01/28/2012	30	Daily
6	2012/13	Santa Maria	09/22/2012	75	Daily
7	2012/13	Santa Maria	11/03/2012	90	Daily
8	2012/13	Santa Maria	12/02/2012	90	Every other day
9	2012/13	Santa Maria	02/06/2013	70	Every other day
10	2013/14	Santa Maria	09/27/2013	86.3	Every other day
11	2013/14	Santa Maria	11/15/2013	110	Every other day
12	2013/14	Santa Maria	02/19/2014	12	Every other day
13	2013/14	Júlio de Castilhos	11/18/2013	N	Twice a week
14	2013/14	Frederico	11/23/2013	N	Twice a week
15	2012/13	Pelotas	11/09/2012	N	Three/week
16	2013/14	Restinga Seca	11/15/2013	N	Twice a week
17	2013/14	Itaqui	10/16/2013	N	Twice a week
18	2013/14	Itaqui	11/24/2013	N	Twice a week
19	2013/14	Itaqui	12/11/2013	N	Twice a week
20	2013/14	Água Santa	12/03/2013	N	Each 10 days
21	2013/14	Tupanciretã	11/17/2013	N	Once a week

<sup>1</sup> - Frequency of phenological measurements (R1, R3, R5 and R7); NM – Irrigated but not measured. N - Experiments conducted under rainfed conditions. In the experiments 1 and 2 plants were manually irrigated with a hose but the amount of irrigated water was not computed and not used in the simulations.

The experiments (irrigated conditions) were irrigated using a drip irrigation system and the amount of irrigated water was computed and used as an input in the model simulations. Each replication was a plot with 15 rows, each row with 3 meters long and 0.45 meters among rows (density of 30 plants.m<sup>-2</sup>). The number of sampled plants varied from 1 to 30 plants, depending upon the experiment and the variable (Table 2).

**Table 2:** Number of samples used for final leaf number (LN), canopy height (CH), per grain dry mass (PG), grain number per m<sup>2</sup> (GN), leaf area index (LAI) and yield (Yi).

Experiment	LN	CH	PG	GN	LAI	Yi
1	19	20	-	-	-	-
2	15	15	-	-	-	-
3	17	18	20	-	-	-
4	19	20	19	-	-	-
5	19	20	20	-	-	-
6	18	20	20	-	-	-
7	18	20	17	-	-	-
8	19	20	20	-	-	-
9	19	20	20	-	-	-
10	16	10	3	3	4	3
11	16	16	4	4	4	4
12	17	20	4	4	4	4
13	21	30	3	3	3	3
14	19	18	4	4	-	4
15	12	11	4	4	4	4
16	10	20	1	1	3	1
17	20	20	4	4	4	4
18	19	19	4	4	4	4
19	20	20	4	4	-	4
20	4	20	1	1	3	1
21	10	20	1	1	3	1

In order to expose the crop model to a wider range of environmental conditions as possible, several experiments were sown outside the recommended sowing period (before and after) which is from mid-October to mid-December, with the best sowing period being from mid-October to mid-November. Sowing dates before October and after December are very early and very late, respectively. Most of cultivars that are grown in the state are in maturity groups V to VII. The cultivar NA5909 RG (maturity group-VI) was selected because it has been one of the most cultivated soybean cultivar across the State during the past four years (2011-2014).

The phenological stages were measured using the scale described by Fehr and Caviness (1977). There are four main developmental stages used in the CROPGRO-Soybean model as

follows: R1 (beginning bloom: plants have at least one open flower at any node), R3 (beginning pod: pods are 5 mm long at one of four uppermost nodes of the main stem), R5 (beginning seed: 33 mm-long seed in the pod at one of the four uppermost nodes of the main stem), R7 (beginning maturity: one normal pod at the main stem attains its mature pod color).

To take advantage of the large number of measurements and to discover how much variability the model is capable of reproducing, all of the observations listed in Table 2 were used, rather than the average values. Therefore, the error was calculated, using the simulated value against each one of the variable observation.

## **2.2 Climate and soil data**

Rio Grande do Sul is the southernmost state of Brazil, with an area of 281,748 km<sup>2</sup>. According to the Köppen system (Köppen, 1931), the climate in this region is classified as subtropical and temperate (Cfa and Cfb), with rain well distributed throughout the year and a mean annual rainfall varying between 1,000 and 2,200 mm (Becker et al., 2012). There are twelve different classes of soils across the state, varying from very deep soils (more than 4.50 m) to shallow soils (less than 1 m) (Streck et al., 2008).

### **2.2.1 Climate data**

Weather data for the experiments conducted in Santa Maria, Pelotas, Julio de Castilhos and Frederico Westphalen were from automatic weather stations located 100 - 150 meters from the trials. For the other locations, weather data were from the closest available automatic weather stations: 15 km from Tupanciretã, 15 km from Restinga Seca, 40 km from Água Santa and 90 km from Itaqui.

Daily data of solar radiation (SRad), maximum and minimum air temperature (Tmax and Tmin) and precipitation (Accum Precip) were used. For the experiments conducted in Tupanciretã and Restinga Seca, the precipitation dataset from the weather stations, were replaced by the recorded precipitation data measured in the fields by local farmers. The weather information used in each of the 21 experiments are summarized as the average cropping season values in Table 3.

**Table 3:** Mean of meteorological conditions (SRad = solar radiation, TMax = maximum temperature, TMin = minimum temperature and Accum Precip = accumulated precipitation). Values are shown for 21 independent experiments were conducted across the State of Rio Grande do Sul.

Weather station (crop season)	SRad (MJ/m <sup>2</sup> )	Tmax (°C)	Tmin (°C)	Accum Precip (mm)	Experiments
Santa Maria (10/11)	20.6	29.4	18.6	568	1
Santa Maria (10/11)	18.3	28.3	17.6	527	2
Santa Maria (11/12)	22.1	29.8	17.4	619	3
Santa Maria (11/12)	21.8	30.9	18.0	467	4
Santa Maria (11/12)	17.0	28.3	15.7	439	5
Santa Maria (12/13)	20.5	28.5	17.4	1096	6
Santa Maria (12/13)	20.8	29.1	17.9	942	7
Santa Maria (12/13)	19.7	28.4	17.4	935	8
Santa Maria (12/13)	13.8	24.7	14.0	564	9
Santa Maria (13/14)	22.1	28.2	16.2	787	10
Santa Maria (13/14)	21.7	28.6	16.8	778	11
Santa Maria (13/14)	11.7	22.7	13.4	1034	12
Julio de Castilhos (13/14)	21.7	30.5	17.1	598	13
Frederico Westphalen (13/14)	22.1	30.0	18.6	758	14
Pelotas (12/13)	20.3	28.2	17.6	628	15
Restinga Seca (13/14)	21.8	28.6	16.8	662	16
Uruguaiana (13/14)	24.1	30.6	18.7	1002	17
Uruguaiana (13/14)	22.9	30.8	19.1	694	18
Uruguaiana (13/14)	22.1	30.5	18.8	560	19
Passo Fundo (13/14)	21.1	28.4	16.9	830	20
Julio de Castilhos (13/14)	21.7	30.5	17.0	831	21

## 2.2.2 Soil data

In the beginning of the soybean project (10/11), the team did not know about the CROPGRO-soybean model soil information requirements (deeper layers), then, the soil physical analysis were sampled only from 0 to 20 centimeters depth. So, the deeper soil layers information were obtained from a survey of natural resources conducted throughout the country in 1986 by the RADAMBrasil project (<http://docslide.com.br/documents/projeto-radambrasil-v33.html>).

After merging the texture class of each layer obtained through *in situ* soil analysis with the survey data from the RADAMBrasil project, the Saxton method (Saxton et al., 1986) was used to calculate the saturated hydraulic conductivity, saturation point, and bulk density. This method estimates soil hydraulic parameters based on texture class according to the percentage content of clay and sand in each layer (Romero et al., 2012). Field capacity and permanent wilting points were calculated by using pedotransfer functions with specific coefficients for soils in Rio Grande do Sul State, given by Reichert et al. (2009). Summary information for the soils of the experimental sites is in Table 4.

**Table 4:** Overview of the soils properties in the 8 experimental sites of this study.

City	Brazilian Soil Classification	FAO Soil Classification	Soil Texture	Soil		
				Depth (cm)	OM (%)	SLPF***
Santa Maria	Podzolico	Carbic podzols	Loam	120	1.9	0.97
Restinga Seca	Podzolico	Carbic podzols	Loam	115	2.4	0.97
Tupancireta	Latossolo	Xantic ferralsols	Clay	300	2.5	0.96
Frederico	Latossolo	Xantic ferralsols	Clay	530	1.6	0.98
Agua Santa	Latossolo	Xantic ferralsols	Clay	380	3.0	0.98
Julio Castilhos	Latossolo	Xantic ferralsols	Sandy	300	2.9	0.98
Itaqui	Cambissolo	Umbric	Silt	65	1.6	0.85
Pelotas	Planossolo	Sodic planossols	Loam	110	0.5	0.94

\* Texture based on the whole soil profile. \*\* Organic matter measured in the firsts 10 centimeters of soil. \*\*\*Generic soil fertility parameter.

### 2.3 Cross-validation experiment design

According to Thorp et al. (2007), the ability of the model to simulate yields improves as the number of growing seasons used for model optimization increases. It was thus decided to use all the observed values in order to better compare the simulated values with all the observed variability in the field. The leave-one-out (LOO) cross-validation method (Efron and Gong, 1983; Efron and Tibshirani, 1998, Baigorria et al., 2010) is a statistical procedure that allows us to include as many seasons of information as possible. In this study, the cross-validation method was used to estimate the ecotype and specific genetic coefficients of cultivar NA 5909 RG.

The calibration procedure was carried out by first calibrating the ecotype coefficients. Ecotype coefficients are the coefficients located in the \*.eco and \*.spe files, and represent parameters of a group of soybean varieties. The coefficients that were modified in the \*.eco file were PL-EM (Time between planting and emergence - in thermal days) and FL-VS (Time from first flower to last leaf on main stem in photothermal-days). The default values were 3.6 thermal days and 12 photothermal days for PL-EM and LF-VS, respectively. These values were changed in order to increase the emergence and final leaf number accuracy during the simulations.

The CROPGRO-soybean model use different base and Optimum temperatures for vegetative, early reproductive and late reproductive phases. These values following Grimm et al., (1993, 1994), and the default values were 7, 28, 35 (vegetative), 6, 26, 30 (early reproductive) and -48, 26, 34, for base (Tb), optimum 1 (TOpt1) and optimum 2 (TOpt2) temperatures, respectively. Then, in order to improve the model responses to early and late sowing dates, inside the \*.spe file, the cardinal temperatures (base and optimum temperatures) in 0.1 °C up and down steps. These temperatures were modified, because the model underestimates and overestimates the vegetative durations of early and late sowing dates, respectively.



To estimate the cardinal temperatures 15 experiments were selected, because they were the ones that had more than one planting date in the same growing season. These 15 experiments also were used to estimate the CSDL (critical short day length) and PPSEN (Slope of the relative response of development to photoperiod with time) genetic coefficients, that locates inside the specific cultivar coefficients \*.CUL file. These coefficients represent each soybean variety in terms of development and growth coefficients. The CSDL and PPSEN coefficients affect mainly the flowering and maturity simulations dates, respectively. These coefficients were changed using 0.1 and 0.01 up and down steps for CSDL and PPSEN, respectively.

Then, after the calibration procedure calibrate the emergence simulations (PL-EM) using all the 21 experiments, the specific genetic coefficients (\*.CUL file) that simulates development and the growth simulations started to be calibrated (Table 5) at 0.1 step increase and decrease from the default value for each coefficient. The range of tested values for each genetic coefficient are shown in Table 5.

**Table 5:** Ecotype, development and growth genetic coefficients were that changed during calibration/validation procedure and their respective ranges.

<b>Coefficients</b>	<b>Description</b>	<b>Range tested</b>	
<b>Ecotype coefficients</b>			
PL-EM	Time between sowing date and plant emergence V0 (thermal days)	2.0	5.0
Tb	Base temperature below which no development occurs (Tb1-vegetative development (VD), Tb2-early reproductive (RD)).	5	11
TOpt1 (VD)	First optimum temperature at which maximum development rate occurs.	25	31
TOpt1(RD)	First optimum temperature at which maximum development rate occurs.	25	29
FL-VS	Time from first flower to last leaf on main stem (photothermal days)	8.0	29

### Development genetic coefficients

CSDL	Critical Short Day Length below which reproductive development progresses with no daylength effect (for short day plants) (h)	12.0	13.0
PPSEN	Slope of the relative response of development to photoperiod with time (positive for short day plants) ( $1.h^{-1}$ )	0.30	0.33
EM-FL	Time between plant emergence and flower appearance (R1) (photothermal days)	22.0	25.0
FL-SH	Time between first flower and first pod (R3) (photothermal days)	3.5	5.5
FL-SD	Time between first flower and first seed (R5) (photothermal days)	10.5	13.0
SD-PM	Time between first seed (R5) and physiological maturity (R7) (photothermal days)	32.0	35.0
FL-LF	Time between first flower (R1) and end of leaf expansion (photothermal days)	8.0	29.0

### Growth genetic coefficients

LFMAX	Maximum leaf photosynthesis rate at 30 °C, 350 vpm CO <sub>2</sub> , and high light ( $mg\ CO_2.m^{-2}.s^{-1}$ ).	0.95	1.09
SLAVR	Specific leaf area of cultivar under standard growth conditions ( $cm^2.g^{-1}$ )	290	400
SIZELF	Maximum size of full leaf (three leaflets) ( $cm^2$ )	150	250
XFRT	Maximum fraction of daily growth that is partitioned to seed + shell	0.50	1.00
WTPSD	Maximum weight per seed (g)	0.10	0.22

The cross-validation leave-one-out (LOO) method consisted in leaving out one of the 21 experiments on each calibration (*i.e.*, 21 calibrations were performed for each coefficient using the data from only 20 experiments ( $m-1$ ) at a time). This approach assured independent data sets for validating each calibration until the lowest Root Mean Square Error (RMSE; Janssen and Heuberger, 1995) was found. The RMSE at each calibration was calculated using the following equations.

$$RMSE_{\bar{x}} = m^{-1} \sum_i \sqrt{\frac{\sum_j (O_{ij} - S_i)^2}{n}} \quad (1)$$

$$RMSE_T = \sqrt{\frac{\sum_i \sum_j (O_{ij} - S_i)^2}{n m}} \quad (2)$$

Where  $RMSE_{\bar{x}}$  is the average root mean square error across all the experiments, and  $RMSE_T$  is the total RMSE, which considers each individual observation.  $O$  is the observed and  $S$  is the simulated value in each experiment  $i$ ,  $j$  is each sample inside the experiment  $i$ ,  $n$  is the number of observations in each experiment, and  $m$  is the number of experiments.

At the end of the procedure, a total of  $m$  sets of coefficients and errors were calculated. Then, the coefficient value with the highest frequency (mode) among the computed  $m$  values was retained and the calibration went to the next genetic coefficient. The procedure was repeated for all development and growth genetic coefficients described in Table 5 until all the coefficients were calibrated.

The results using the cross validation approach were compared to the results with the classical approach for calibrating the genetic coefficients of the CROPGRO-soybean model (Garrison et al., 1999; Zhao et al., 2000; Bakhsh et al., 2001). The classical calibration/validation procedure was conducted by using three datasets (experiment 10, 11 and 12), and the remaining 18 experiments (1, 2, 3, 4, 5, 6, 7, 8, 9, 13, 14, 15, 16, 17, 18, 19, 20 and 21), for calibration and validation, respectively. These experiments were selected because they represent a wide range of sowing dates inside the same crop season (very early, optimum and very late sowing dates).

### **3. RESULTS AND DISCUSSION**

#### **3.1 CROPGRO-soybean genetic Coefficients**

In order to increase the accuracy of very early and late sowing dates simulations, the default values were changed for the estimated values that showed the lowest RRMSE's. The estimated new values were 10°C, 8°C, 29°C and 28°C, for vegetative and early reproductive base (Tb1 and Tb2) and optimum temperatures (TOpt1 and TOpt2), respectively. The genetic coefficients (Table 5) for cultivar NA 5909 RG values estimated through calibration/validation procedure for CSDL and PPSEN were 12.71 hours and 0.310 hour<sup>-1</sup>, respectively.

The ecotype coefficient PL-EM and the cultivar specific development and growth genetic coefficients are shown in Table 6. The estimated development genetic coefficient FL-LF was 26 photothermal days. The estimated growth genetic coefficients were 1.000 mg.CO<sub>2</sub>/m<sup>2</sup>.s, 355 cm<sup>2</sup>/g, 220 cm<sup>2</sup> and 0.17 g for LFMAX, SLAVR, SIZELF and WPSD, respectively.

**Table 6:** Development genetic coefficients estimated through cross-validation calibration/validation procedure and the respective root mean square error's obtained for each one of the 21 validations.

Estimated	PL-EM	EM-FL	FL-SH	FL-SD	SD-PM
	3.4	23.4	5.0	11.6	34.1
Experiment	Emergence	Average RMSE's (days).			
		R1	R3	R5	R7
1	0.975	4.135	4.135	6.321	6.021
2	1.162	4.207	4.105	6.321	6.281
3	1.162	4.231	4.062	6.181	6.281
4	1.095	4.177	3.854	6.181	6.423
5	1.162	4.231	4.159	6.321	6.325
6	1.183	4.177	3.854	5.362	6.419
7	1.183	3.931	4.105	6.289	6.325
8	1.183	4.231	4.153	6.325	6.325
9	1.183	4.231	4.153	6.289	6.325
10	1.095	4.225	4.159	6.225	6.021
11	1.162	4.225	4.105	6.128	6.423
12	1.162	3.931	3.354	5.000	6.099
13	1.162	4.080	4.153	6.321	6.168

14	1.162	4.080	4.105	6.261	6.281
15	1.162	4.231	4.062	6.261	6.281
16	1.183	4.207	4.153	6.128	6.325
17	1.162	4.231	4.153	6.181	6.325
18	1.183	3.722	4.105	6.321	6.021
19	1.162	3.931	4.105	6.325	6.229
20	1.162	4.231	4.062	6.325	6.423
21	1.183	4.012	4.062	6.325	6.281

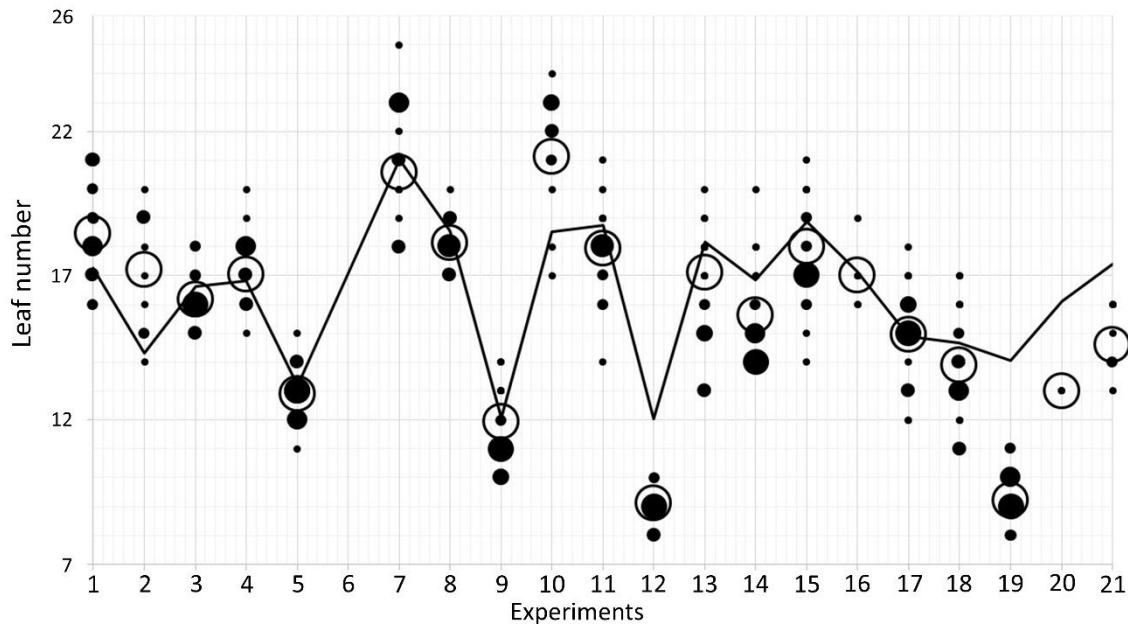
In general, the emergence, R1, R3, R5 and R7 RMSEs varied from 0.975 to 1.183 days (average of 6 DAS (Days After Sowing)), 3.722 to 4.231 days (average of 52 DAS), 3.354 to 4.159 days (average of 64 DAS), 5.000 to 6.325 days (average of 77) and 6.021 to 6.234 (average 124 DAS), respectively. Considering the wide variability of sowing dates, the simulations showed reasonable agreement between the observed and simulated values (correlation  $r$  of 0.73, 0.87, 0.89, 0.85 and 0.87) for emergence, R1, R3, R5 and R7, respectively. Pedersen et. al. (2004), using a sowing date range that comprising only one month (May) in the South and middle of Wisconsin State, U.S., found 2.9 and 2.5 days for emergence and R1 RMSEs, respectively. Mercau et. al. (2007), using sowing dates from October 1 to January 10, in Argentine Pampas (near from RS), found 7, 9 and 10 days for R1, R5 and R7 RMSEs, respectively. Then, even considering a wider sowing date range, the results obtained in this study, showed higher accuracy than in other studies. For the growth parameters, several experiments did not have all the observed data. The RMSEs calculated during the growth coefficients calibration are shown in Table 7.

**Table 7:** Calculated  $RMSE_{\bar{x}}$  ( $\bar{x}$ ) and  $RMSE_T$  ( $T$ ) by using the cross-validation method in all experiments

EXP	Leaf Number		LAI Index		Canopy height (m)		One grain (g)		Grain number (gains.m <sup>-2</sup> )		Yield (kg.ha <sup>-1</sup> )	
	$\bar{x}$	$T$	$\bar{x}$	$T$	$\bar{x}$	$T$	$\bar{x}$	$T$	$\bar{x}$	$T$	$\bar{x}$	$T$
1	2.55	3.33	N	N	0.23	0.26	N	N	N	N	N	N
2	2.54	3.30	N	N	0.24	0.26	N	N	N	N	N	N

3	2.62	3.36	N	N	0.23	0.26	0.03	0.04	N	N	N	N
4	2.60	3.36	N	N	0.24	0.26	0.03	0.04	N	N	N	N
5	2.62	3.38	N	N	0.24	0.26	0.03	0.04	N	N	N	N
6	2.61	3.33	N	N	0.22	0.25	0.03	0.04	N	N	N	N
7	2.58	3.34	N	N	0.22	0.25	0.03	0.04	N	N	N	N
8	2.62	3.35	N	N	0.23	0.26	0.03	0.04	N	N	N	N
9	2.61	3.37	N	N	0.24	0.26	0.03	0.04	N	N	N	N
10	2.48	3.26	1.34	1.56	0.22	0.24	0.03	0.04	272	372	375	461
11	2.58	3.35	1.29	1.67	0.22	0.25	0.03	0.04	340	514	424	557
12	2.55	3.33	1.36	1.71	0.24	0.26	0.03	0.04	345	522	426	555
13	2.60	3.36	1.26	1.63	0.23	0.26	0.03	0.04	361	528	463	591
14	2.56	3.34	N	N	0.23	0.26	0.03	0.04	369	531	433	568
15	2.55	3.33	1.09	1.30	0.23	0.26	0.03	0.04	314	469	434	567
16	2.61	3.31	1.27	1.64	0.23	0.26	0.03	0.04	373	515	468	578
17	2.44	3.19	1.35	1.70	0.23	0.25	0.03	0.04	345	527	477	607
18	2.40	3.11	1.32	1.69	0.23	0.26	0.03	0.04	373	541	468	603
19	2.24	2.57	N	N	0.23	0.25	0.03	0.04	371	541	474	602
20	2.49	3.28	1.30	1.66	0.24	0.26	0.02	0.03	367	514	481	579
21	2.50	3.28	1.20	1.57	0.24	0.26	0.03	0.04	343	510	445	573

The observed final leaf number varied among experiments and so did the model (Figure 2) with an average RMSE of 2.5 leaves and a correlation of 0.85 between the average observed and simulated leaf number. Which means that despite some poor performances (experiment 10 and 12), the model showed good ability to simulate the final leaf number variability among the experiments.



**Figure 2:** Simulated (line) and observed (dots) final leaf number in the main stem on each experiment. Dot size varies according to the number of observations. Hollow circles indicates the observed average.

Despite mimicking the trend in the experiments 1 and 2, the model clearly underestimated the final leaf number. These errors could be partly explained, by the fact that the model was run for rainfed conditions (the model simulated water stress, which decreased the final leaf number). The experiment was irrigated a few times, but the amounts were not measured (Table 1), which did not allow to input the irrigated water into the model simulations.

The simulated R1, R3 and R5 stage in the experiment 10 were very closer to the observed values, which means that the model reproduced well the vegetative and reproductive development. The simulated and average observed final leaf number were 18 and 21 leaves, respectively. However, Martins et al. (2011), using 15 soybean cultivars (three sowing dates: beginning of November, December and January) in Santa Maria (RS) Brazil, found a decrease of final leaf number with delay in sowing dates. The average cultivars final node number and plastochron were

22, 18 and 14 nodes and 59, 51 and 50  $C^{\circ} \cdot \text{node}^{-1}$  for first, second and third sowing dates, respectively.

In order to find the final leaf number underestimation cause in the experiment 10, the leaf appearance equation was checked. According to this equation, the same rate of appearance of leaves per thermal day (TRIFL) was used for all the 21 experiments. Then, the low observed air temperatures in the beginning of the spring simulated a lower final leaf number in the experiment 10. This effect was enhanced by water stress occurred before the irrigation system was ready (Figure 3). On the other hand, the model overestimated the experiment 12 final leaf number, which is a too late sowing date (February 19). According to the simulation daily results, there was no water stress in this experiment (Figure 3).

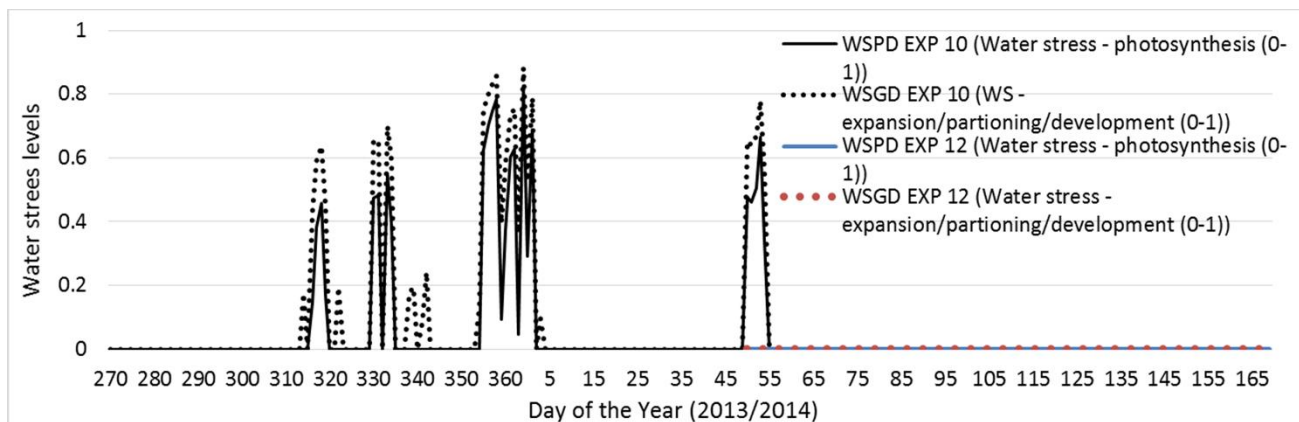


Figure 3: Simulated daily water stress during the experiment 10 period in the field.

However, the same leaf appearance rate was used and the higher February temperatures increased the simulated final leaf number. This effect was enhanced by an increase in simulated phenological stages duration, the model simulated the R1, R3 and R5 stages with 7, 12 and 17 days longer than the observed, respectively.



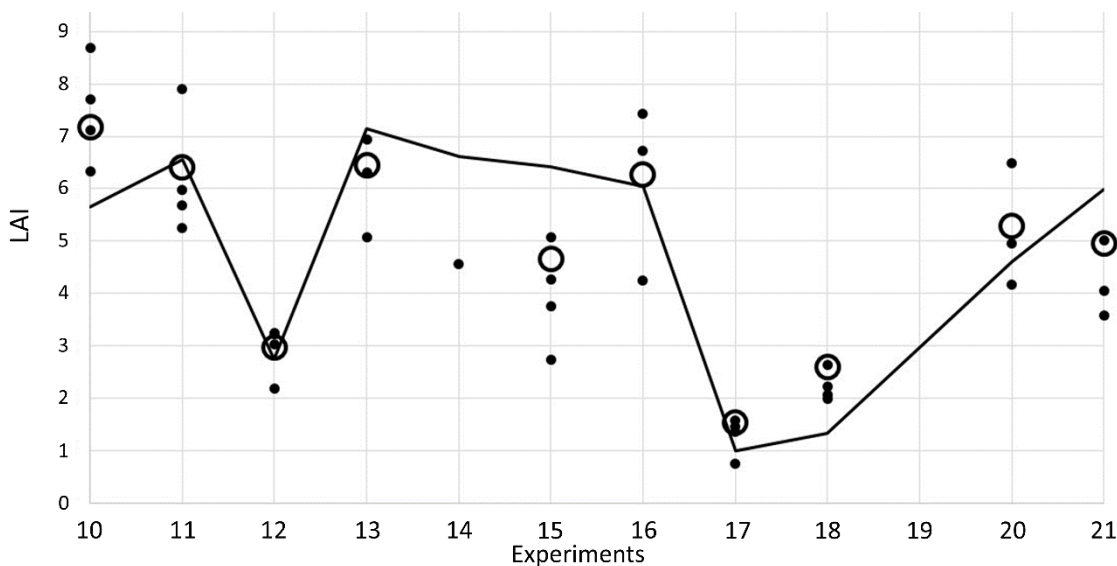
Curiously, in the experiment 9 (an also late sowing date) sown on February 6, the solar radiation and temperature were lower ( $14.6^{\circ}\text{C}$  ;  $13.4 \text{ MJ m}^{-2}$ ) than during normal planting dates ( $22.5^{\circ}\text{C}$  and  $18.3 \text{ MJ m}^{-2}$ ). The opposite pattern occurred with precipitation (529 mm versus 737 mm); however, the model still simulated the same number of leaves of the experiment 12. Additionally, the model showed a delay of five and six days for the R1 and R3 stages, respectively, which lengthened the vegetative and early reproductive phases and consequently lengthened the simulated leaf appearance period.

The Itaqui region (the most West experiments 17, 18, and 19) is and outside soybean agro-climatic zoning system (MAPA), and farmers in this region grow soybeans mainly to reduce weeds, control pest problems and increase soil fertility in rice cropping systems. The model had difficult to reproducing the leaf number for the late sowing (December sowing). The model estimate delayed R1 by seven days and allowed the plant to develop more leaves than observed. Moreover, the weather station is located 100 kilometers away from the experimental site, which could have added uncertainty. So, despite to show a good variability agreement in almost all the experiments, the model showed a low performance to correct represent the early and late sowing dates final leaf number variability (experiment 10, 12 and 19). Finally, the simulated leaf numbers for experiments 20 and 21 were higher than observed, which could be attributed to weather data taken from a weather station located far from the experimental sites. Additionally, the site for experiment 20 is the farthest, decreasing the observation frequency (10 days) and unfortunately the R1, R5, and R7 dates were missed.

The leaf area index (LAI) was the second growth parameter to be calibrated, and the model showed an LAI average RMSE and correlation of 1.28 and 0.78 (Figure 4). The large LAI

difference in experiment 15 is explained by a caterpillar attack observed during the grain filling stage.

The same effect observed in Figure 3 is shown in Figure 4 after cross-validation was applied, and there were model simulations underestimations in LAI and FLN in the experiment 10. The only exception occurred with experiment 15 due to the difference between the observed and simulated LAI. When experiment 15 was removed from consideration, the RMSE significantly dropped to 1.09 (Table 7). For comparison, with independent datasets in central Missouri, the CROPGRO-soybean model simulated LAI with an overall RMSE of 1.07 (Wang et al., 2003).

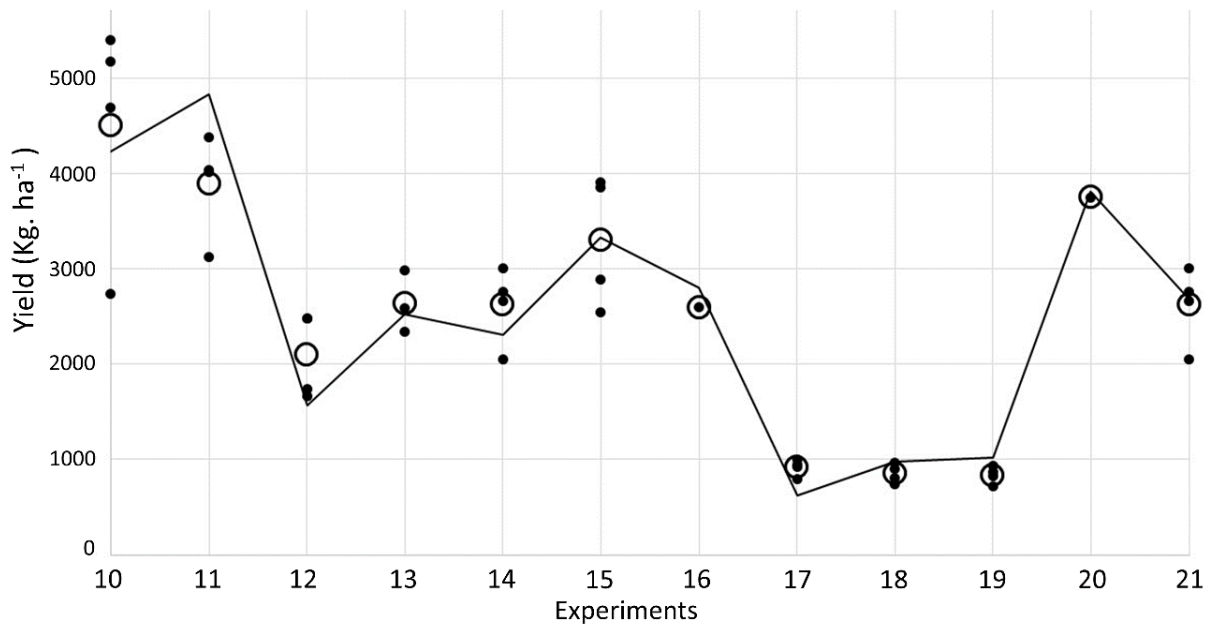


**Figure 4:** Simulated (line) and observed (small dots) LAI on each experiment. Empty circles= average observed LAI.

The calculated averaged RMSEs for the simulated canopy height and one-grain dry mass values ranged from 20 to 22 centimeters and from 20 to 30 milligrams, respectively, showing a very similar behavior in all the cross-validation results.

The RMSE for grain number varied from 272 to 373 grains.m<sup>-2</sup> and for yield, the variation was from 375 to 481 kg.ha<sup>-1</sup> (Table 7). These results were very reasonable if compared with the ones found by Setiyono et al., (2010b) (RMSEs of 625 grains.m<sup>-2</sup> and 460 kg.ha<sup>-1</sup>).

These results suggest that the errors were reasonably distributed over the 11 experiments (Figure 5). According to Table 7,  $RMSE_T$  was always higher than  $RMSE_{\bar{x}}$  indicating that by giving the same value to all of the observations in each experiment, the  $RMSE_T$  was more exposed to the observed variability than the  $RMSE_{\bar{x}}$ .



**Figure 5:** Simulated (line) and observed (small dots: replication samples; empty circles: observed average grain yield) grain yield on each experiment.

Finally, a comparison between the classical and the cross-validation calibration/validation approach showed significant improvements in most part of the parameters. The phenological average RMSE decreased from 2.6, 4.6, 4.8, 7.3 and 10.2 days using the classical calibration to 1.1, 4.1, 4.1, 6.2 and 6.3 days using the cross-validation for EM-FL, FL-SH, FL-SD and SD-PM stages, respectively. The increase in simulations precision can improve the efficiency of decision

making of the crop/farm management, with a better accurate phenological and grain yield estimative.

In the growth parameters, the cross validation method also improved the average RMSE from 1.40, 0.29, 677 and 551 to 1.30, 0.39 grams, 347 and 447 for LAI, grams (one grain dry mass), grains.m<sup>-2</sup> and kg.ha<sup>-1</sup>, respectively. On the other hand, the cross validation worsened the average RMSE from 2.1 and 0.21 to 2.5 leaves and 0.23 meters for final leaf number and canopy height, respectively.

It is also important to highlight that alterations in the sowing date could greatly change the relationship of any given variety to average conditions (Irmak et. al. 2000). Thus, the performance of CROPGRO-soybean could be further improved, as the early and late sowing dates were primarily responsible for the differences between observed and simulated phenology stages (DAS).

#### **4. CONCLUSIONS**

The coefficients calculated through the cross-validation method generally resulted in a better performance of the model than the classical procedure. Compared to the classical calibration/validation procedure, these optimum coefficients improve the model capabilities to simulating the variability among the different environment conditions. In addition, there were only two parameters that the cross-validation method showed worsts results (final leaf number and canopy height).

The CROPGRO-soybean R7 stage estimation accuracy for example, was improved in four days. Furthermore, there were no significant differences among the optimum genetic coefficients

estimated from each one of the 21 cross-validation runs (very low value differences). In other words, there were stability among the estimated ecotype and genetic coefficients across the studied regions of the State in normal sowing season (the variety NA 5909, showed homogeneous behavior even considering a wide range of environment conditions and sowing dates).

It is also important to highlight that the CROPGRO-soybean model provided robust predictions of phenology, biomass and yield components variability considering the wide range of environment conditions and sowing dates. Finally, we can conclude that to improve the ecotype and genetic coefficients estimation, the model performance and the efficiency of experiment number use, the cross-validation LOO method should be used whenever possible.

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**6 ARTIGO 2**

**ON THE NUMBER OF EXPERIMENTS REQUIRED TO CALIBRATE A CULTIVAR  
IN A  
CROP MODEL: THE CASE OF CROPGRO-soybean.**

(Artigo publicado na revista Field Crops Research)



**ON THE NUMBER OF EXPERIMENTS REQUIRED TO CALIBRATE A CULTIVAR  
IN A  
CROP MODEL: THE CASE OF CROPGRO-soybean.**

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**Abstract**

The conventional approach for calibrating/validating a crop model considers few to many experiments. However, few experiments could lead to higher uncertainties and a large number of experiments is too expensive. The objectives of this research were to study the calibration uncertainties and to find out the minimum number of experiment required for a reliable CROPGRO-Soybean model calibration. This study uses 21 field experiments (BMX Potencia RR variety) sown in eight different locations of Southern Brazil between 2010 and 2014. The experiments were grouped in four classes (Individual sowings, season/year per location, experimental site and all data together). The developmental RRMSE (%) decreased from 22.2% to 7.8% in individual sowings to all data together classes, respectively. Use only an individual sowing to calibrate the model, could lead to a RRMSE of 28.4, 48, and 36% for R1, LAI and yield, respectively.

*Key words:* CROPGRO-soybean, genetic coefficients, uncertainty, cross-validation, optimization

**1. INTRODUCTION**

Crop models are widely used in agriculture research to extrapolate the performance of genotypes under varying growing conditions. The CROPGRO-soybean is the model in the Decision Support System for Agrotechnology Transfer (DSSAT) system for simulating soybean crop growth and development (Jones et al., 2003). During the last 25 years, soybean area and production in Brazil have increased remarkably with six-fold more production and three times expansion in cultivation area (USDA-FAS, 2015). This expansion in soybean cultivation and its

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contribution to the country economy have drawn government as well as private sector attentions. This expansion increased the economic and competitive pressure, leading to soybean companies to increase their variety release rate and making variety characterization a challenge to the soybean developers. Furthermore, the rapid release of new cultivars makes multi-locations trials a priority compared to multi-years trials to evaluate the performance of the cultivar in multiple climate, management, soil and cropping system (Welch et al., 2002). This task is even more challenging to non-profit organizations like universities, research institutes and independent researchers who intent to test new technologies under diverse environmental conditions as these field evaluations are time-consuming, laborious and expensive.

To cope with this problem, the ability of crop models to test the particular genotypes in various growing conditions without conducting field research are being explored in recent years. However, the reliability of crop models for simulating crop growth and yield under different environments is uncertain. One of the major factors for the success is its calibration process (Ruíz-Nogueira et al., 2001, Xiong et al., 2014), which determines the applicability of model on a larger scale (Angulo et al., 2013). CROPGRO-soybean has been calibrated and evaluated using datasets from one experiment to a combination of many experiments conducted at various locations, years, sowing dates and other management practices (Boote et al., 1997, Irmak, 2001).

Crop growth, development and yield are dependent on growing conditions. Thus, a single experiment can only represent a particular production environment. Therefore, information from one experiment to estimate genetic coefficients and to calibrate an entire model might not be sufficient to simulate crop yield for other environments. Moreover, multiple experiments with a large amount of observed data, usually uses only optimum or near-optimum sowing dates, which

also could lead to improper model calibration. The number of samples for each growth and development parameter could also have effect on the reliability of the model.

This study aims to evaluate the uncertainties caused by field experiments during variety calibration and to estimate the optimum number of experiments required for a more reliable calibration and validation of the CROPGRO-Soybean model.

## **2. DATA AND METHODS**

### **2.1 Field experiment data**

The data comprised four growing seasons of field experiment (2010/2011- 2013/2014) conducted at eight different locations in the Rio Grande do Sul (RS) State (Figure 1). The experiments started at Santa Maria in 2010/2011 and gradually replicated to other regions. Each experimental site represent different soybean growing region of the State. Tupancireta and Julio de Castihos rank as the first and the third larger soybean grown area in the state. Agua Santa represents the most soybean productive region. In Itaqui and Pelotas, farmers are growing soybean only to fit in their crop rotations with irrigated rice in lowlands, to reduce weed infestation and improve soil fertility. Frederico Westphalen is located in high frequency drought region, and in this region it is common a shift towards early and late sowing dates. This shifts allows growing two summer crops per year (Zanon et al., 2016). Santa Maria and Restinga Seca are mostly counties with small farming systems. Out of thirteen different soybean varieties, BMX Potencia (Maturity group VI) was chosen for this study. This cultivar was the most planted soybean genotype in the south of Brazil in past three years (2012-2014).

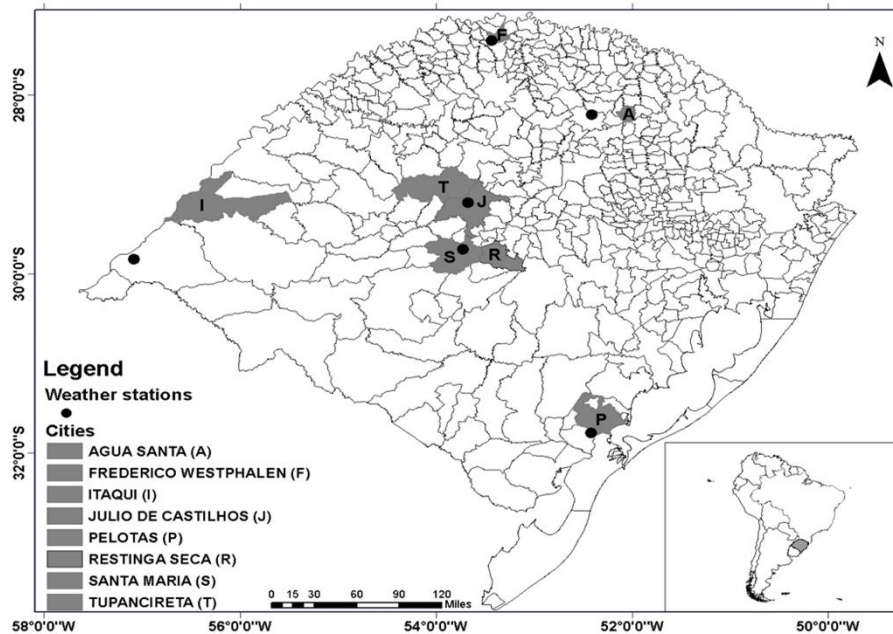


Figure 1: Experimental sites conducted across the Rio Grande do Sul State (Grey polygons) and the closest weather stations were used to each site simulation.

The experimental design was a complete randomized block, with four replications. Each replication was a plot with 15 rows, each row with 3 meters long and 0.45 meters between rows (plant density of 31/m<sup>2</sup>). The soybean developmental stages R1 (beginning bloom), R3 (beginning pod), R5 (beginning seed) and R7 (beginning maturity) were measured according to the Fehr and Caviness (1977) scale. The final leaf number was obtained when the leaf appearance stopped and the Leaf area index (LAI) was measured twice a month. The canopy height was measured when the plants were ready to be harvested (R8). The number of grains per meter square was counted at the harvest and also a sample with a hundred grains was separated and oven dried at 60 °C to determine the dry mass of one grain. Finally, the grain yield was obtained on a 13% moisture basis. The detailed information on seasons, locations, sowing dates, irrigation records, measurements interval and observation intervals are in Table 1, Richter et al., 2014 and Zanon et al., 2015 a, b.

**Table 1:** Experiments with soybean conducted during four growing seasons (2010/2011, 2011/2012, 2012/2013 e 2013/2014) at eight locations in the state of Rio Grande do Sul, Brazil.

Experiment	Location	Crop season	Sowing date	Sowing time	Irrigation (mm)	Measurement interval <sup>1</sup>
1	Santa Maria	2010/11	12/10/2010	Optimum	N	Daily
2	Santa Maria	2010/11	01/08/2011	Late	N	Daily
3	Santa Maria	2011/12	09/24/2011	Early	193	Daily
4	Santa Maria	2011/12	11/19/2011	Optimum	130	Daily
5	Santa Maria	2011/12	01/28/2012	Late	30	Daily
6	Santa Maria	2012/13	09/22/2012	Early	75	Daily
7	Santa Maria	2012/13	11/03/2012	Optimum	90	Daily
8	Santa Maria	2012/13	12/02/2012	Optimum	90	Alternate day
9	Santa Maria	2012/13	02/06/2013	Late	70	Alternate day
10	Santa Maria	2013/14	09/27/2013	Early	86.3	Alternate day
11	Santa Maria	2013/14	11/15/2013	Optimum	110	Alternate day
12	Santa Maria	2013/14	02/19/2014	Late	12	Alternate day
13	Julio de Castilhos	2013/14	11/18/2013	Optimum	N	Twice a week
14	Frederico	2013/14	11/23/2013	Optimum	N	Twice a week
15	Pelotas	2012/13	11/09/2012	Optimum	N	Three times a week
16	Restinga Seca	2013/14	11/15/2013	Optimum	N	Twice a week
17	Itaqui	2013/14	10/16/2013	Optimum	N	Twice a week
18	Itaqui	2013/14	11/24/2013	Optimum	N	Twice a week
19	Itaqui	2013/14	12/11/2014	Late	N	Twice a week
20	Agua Santa	2013/14	12/03/2013	Optimum	N	Each 10 days
21	Tupancireta	2013/14	11/17/2013	Optimum	N	Once a week

<sup>1</sup> Frequency of phenological measurements (R1, R3, R5 and R7);

N – Experiments conducted under rainfed conditions.

## 2.2 Climate and soil data.

The Rio Grande do Sul lies in southern part of Brazil. The climate is humid subtropical with 86.7 percent with hot summer (Cfa) and 13.3 percent with temperate summer (Cfb) based on Köppen system climate classification (Alvares et al., 2013).

### 2.2.1 Climate data

The daily weather data for maximum and minimum temperature (TMax and TMin) solar radiation (SRad) and precipitation (Rain) used in this study were collected from National Institute

of Meteorology (INPE), Brazilian Agriculture Research Corporation (EMBRAPA) or Foundation of livestock and agriculture research of the State (FEPAGRO). Since all the experimental sites do not have weather stations, especially Agua Santa, Itaquí and Tupancireta, most nearest weather stations, Passo Fundo, Uruguai and Julio de Castilhos station weather data has been used, respectively. The details on seasonal weather average prevailed were listed in Table 2.

**Table 2:** Average of meteorological conditions (Srad = solar radiation, TMax = maximum temperature, TMin = minimum temperature and Total Rain = accumulated precipitation) during the experiments with soybean in the State of Rio Grande do Sul, Brazil.

Weather station	Experiments	SRad (MJ/m <sup>2</sup> )	TMax (°C)	TMin (°C)	Total Rain (mm)
Santa Maria 10/11	1	20.6	29.4	18.6	568
Santa Maria 10/11	2	18.3	28.3	17.6	527
Santa Maria 11/12	3	22.1	29.8	17.4	619
Santa Maria 11/12	4	21.8	30.9	18.0	467
Santa Maria 11/12	5	17.0	28.3	15.7	439
Santa Maria 12/13	6	20.5	28.5	17.4	1096
Santa Maria 12/13	7	20.8	29.1	17.9	942
Santa Maria 12/13	8	19.7	28.4	17.4	935
Santa Maria 12/13	9	13.8	24.7	14.0	564
Santa Maria 13/14	10	22.1	28.2	16.2	787
Santa Maria 13/14	11	21.7	28.6	16.8	778
Santa Maria 13/14	12	11.7	22.7	13.4	1034
Julio de Castilhos	13	21.7	30.5	17.1	598
Frederico Westphalen	14	22.1	30.0	18.6	758
Pelotas	15	20.3	28.2	17.6	628
Restinga Seca	16	21.8	28.6	16.8	662
Uruguai	17	24.1	30.6	18.7	1002
Uruguai	18	22.9	30.8	19.1	694
Uruguai	19	22.1	30.5	18.8	560
Passo Fundo	20	21.1	28.4	16.9	830
Julio de Castilhos	21	21.7	30.5	17.0	831

### 2.2.2 Soil data

The physical characteristics of upper layer top soil (0-20 cm) were analyzed through soil sampling from all sites. Information from deeper layers were obtained traced from RADAMBrasil (1986) project. Following the Global Reanalysis Soil Database Methods (Romero et al., 2012), the Saxton method (1986) was applied to estimate soil bulk density, saturated hydraulic conductivity and saturation point. Further, for the specific soils of Rio Grande do Sul, Reichert et al. (2009) pedotrasfer functions were used to compute permanent wilting point (PWP) and field capacity (FC). The details on soil were presented on Table 3.

Table 3: Overview of the soils properties found in the 8 experimental sites of this study.

City	Brazilian Classification	FAO Classification	Texture*	Depth (cm)	OM (%)**
Santa Maria	Podzolico	Carbic podzols	Loam	120	1.9
Restinga Seca	Podzolico	Carbic podzols	Loam	115	2.4
Tupancireta Frederico	Latossolo	Xantic ferralsols	Clay	300	2.5
Westphalen	Latossolo	Xantic ferralsols	Clay	530	1.61
Agua Santa	Latossolo	Xantic ferralsols	Clay	380	3.0
Julio Castilhos	Latossolo	Xantic ferralsols	Sandy Clay	300	2.9
Itaqui	Cambissolo	Umbric cambissols	Silt Loam	65	1.6
Pelotas	Planossolo	Sodic planossols	Loam	110	0.48

\* Texture based on the whole soil profile.

\*\* Organic matter measured in the firsts 10 centimeters of soil.

### 2.3 Grouping experiments approach

All together, there were twenty-one different experiments resulted from locations, years and sowing dates combinations used in this study. These experiments were organized into four different groups:

#### 2.3.1 Group 1: Individual sowings →

Each of the twenty-one experiments were used to calibrate the model separately, which means one set of genetic coefficients for each sowing date.

#### 2.3.2 Group 2: season/year per location →

The sowing dates within a growing season conducted at a particular location were aggregated. For instance, for Santa Maria, there were four sowing dates in the year 2012/13, thus all the four sowing dates were used to calibrated the phenological and growth genetic coefficients. There were five different field experiment groups with 2 (experiments 1 and 2), 3 (experiments 3, 4 and 5), 4 (experiments 6, 7, 8 and 9), 3 (experiments 10, 11 and 12) and 3 (experiments 17, 18 and 19) experiments (Table 1).

### **2.3.3 Group 3: Experimental sites →**

All the available experiments within a given location were clustered. This included planting dates and growing seasons. There were two groups in this level of aggregation: group one had 12 experiments (1 to 12 conducted at Santa Maria) and group two had 3 experiments (17 to 19 conducted at Itaquí) (Table 1).

### **2.3.4 Group 4: All data together →**

Temporal integration using different planting dates and seasons, and spatial integration using different locations. All available twenty one experiments were used to calibrate the cultivar.

## **2.4 CROPGRO-Soybean Model Setting and Calibration/Validation.**

The CROPGRO-Soybean (Boote et al., 1998) model on DSSAT 4.5 version is one of the most used model in agriculture research field to simulate soybean growth, development and yield (Hoogenboom et al., 2012, Salmerón et al., 2016). In this research, the model was calibrated/validated following a cross-validation method.

The cross-validation leave-one-out (LOO) method (Efron and Gong, 1983; Efron and Tibshirani, 1998, Baigorria et al., 2010) is a statistical procedure that allows to use as many sets of observed experimental data as possible. This method allowed to calibrate/validate 21



experimental datasets (N) in 21 different repetitions (k) ( $N = k$ ). In each k repetition, 20 experimental datasets were used to calibrate and the remaining one to validate as an independent dataset. In the end, each repetition k was conducted without an exclusive experimental dataset until all the 21 experiments were left out once. The calibration/validation procedure always started from EM-PL coefficient and kept advancing until the last one was calibrated (following the sequence in Table 4).

Table 4: Development and growth genetic coefficients used in the calibration/validation procedure.

Coefficient	Description
Development genetic coefficients	
EM-FL	Time between plant emergence and flower appearance (R1) (photothermal days = PD)
FL-SH	Time between first flower and first pod (R3) (PD)
FS-SD	Time between first flower and first seed (R5) (PD)
SD-PM	Time between first seed (R5) and physiological maturity (R7) (PD)
FL-LF	Time between first flower (R1) and end of leaf expansion (PD)
Growth genetic coefficients	
LFMAX	Maximum leaf photosynthesis rate at 30°C, 350 vpm CO <sub>2</sub> , and high light (mg CO <sub>2</sub> / (m <sup>2</sup> - s).
SLAVR	Specific leaf area of cultivar under standard growth conditions (cm <sup>2</sup> /g)
SIZELF	Maximum size of full leaf (three leaflets) (cm <sup>2</sup> )
XFRT	Maximum fraction of daily growth that is partitioned to seed + shell
WTPSD	Maximum weight per seed (g)
PODUR	Time required for cultivar to reach final pod load under optimal conditions (PD)
SFDUR	Seed filling duration for pod cohort at standard growth conditions (PD)

The genetic coefficients were changed manually (trial and error method) by decreasing/increasing the coefficients in a 1 to 10% step depending upon the coefficients. For each k repetition, a set composed by 12 genetic coefficients were determined by minimizing the Relative Root Mean Square Errors (RRMSE):

$$RRMSE = \left( \frac{\sqrt{\frac{\sum (oin-si)^2}{n}}}{\theta} \right) * 100$$

Where  $s$  is the simulated and  $o$  the observed value in each experiment  $i$ ,  $n$  is number of measurements in each variable and  $\theta$  is the average of all observed values. When the calibration/validation procedure was completed, it produced 21 best values for each one of the 12 genetic coefficients, and then, among the 21 values, the most common was considered as the final value of genetic coefficient.

### 3. RESULTS

The 11 genetic coefficients estimated with the cross-validation procedure in each one of the 29 combinations among locations, years and sowing dates are shown in Figure 2 and 3 as box plots. There are only 11 genetic coefficients in the Figures because the genetic coefficient XFRT was not changed during all calibration/validation. Among the genetic coefficients with units of photothermal days (Figure 2), the Individual sowings group showed the higher variability in most coefficients. This variability indicates different responses of a specific soybean variety under different environmental conditions. The wide range among the calibrated genetic coefficients was due to the large range of sowing dates, varying from September to February.

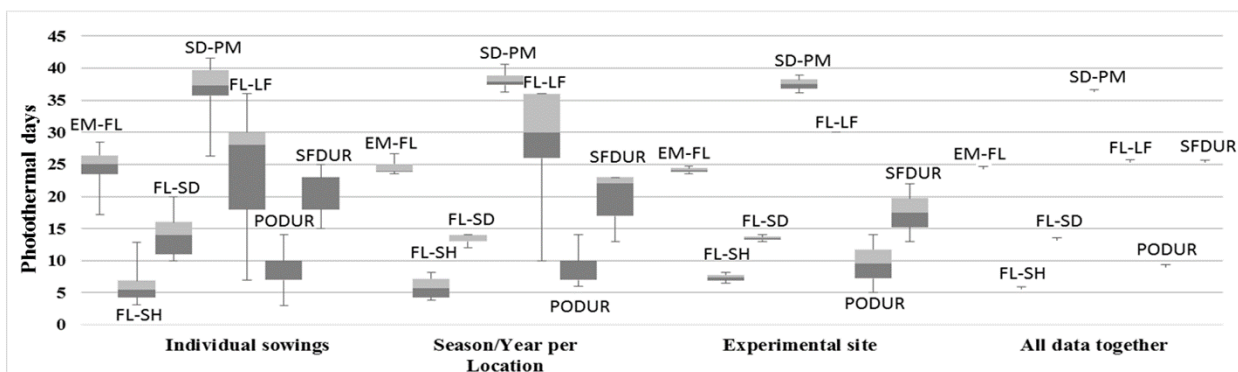


Figure 2: Variability of seven genetic coefficients (described in Table 4: EM-FL, FL-SH, FL-SD, SD-PM, FL-LF, PODUR and SFDUR) of the CROPGRO-soybean model as a function of different groupings of experiments.

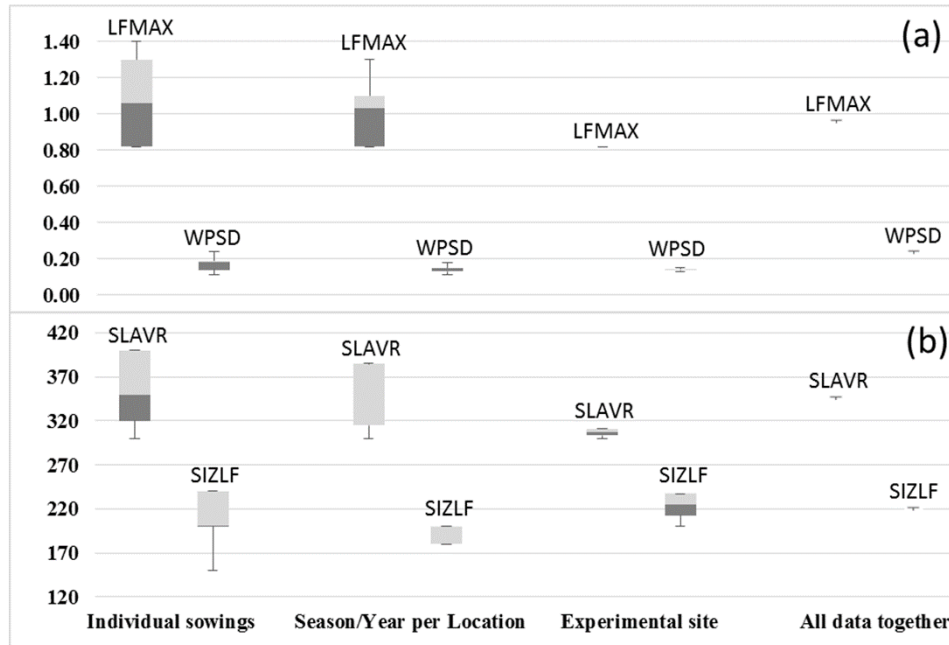


Figure 3: Variability of four genetic coefficients {described in Table 4: LFMAX, WPSD (panel a), and SLAVR and SIZLF (panel b) of the CROPGRO-soybean model as a function of different groupings of experiments.

The genetic coefficients LFMAX, WPSD, SLAVR and SIZLF are presented in Figure 3 because they have different units other than photothermal days. Similarly to trend observed in Figure 2, the Individual sowings group also showed the higher variability in most of coefficients compared to the other groupings, i.e. the range of all growth genetic coefficients also decreased as the aggregation level increased.

The RRMSE calculated in the calibration/validation process using each set of development and growth genetic coefficients were summarized in box plot values on Table 6. As observed in the genetic coefficients variability, the individual sowings group produced the higher range of errors in the simulations. In the phenological stages simulations showed a RRMSE that varied from 4.1% to 28.7%.

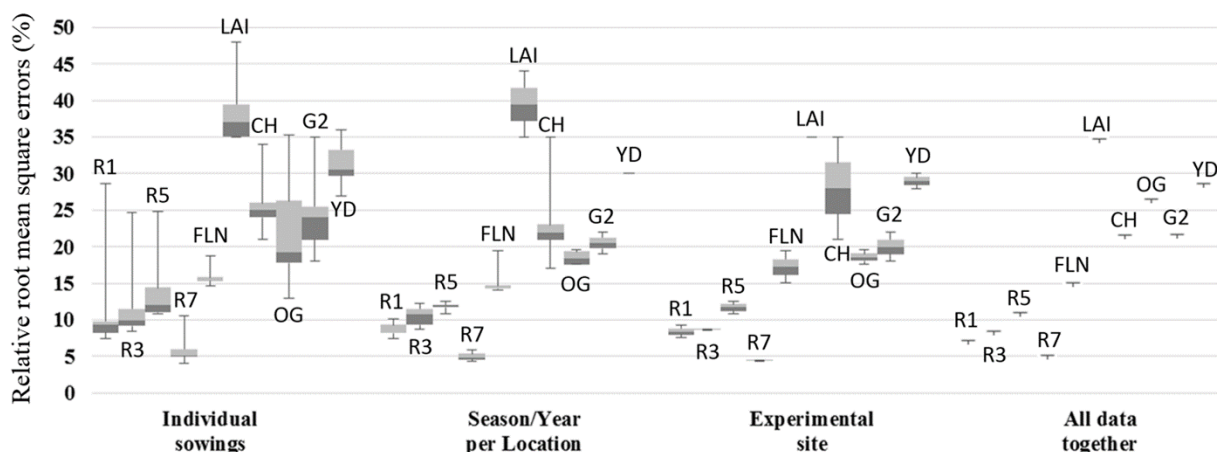


Figure 4: Relative root mean square error (RRMSE %) of developmental stages (R1, R3, R5, R7, and FLN) and growth variables (LAI, Canopy height – C.H., one grain dry mass – O.G., number of grains per meter square – G2, and grain yield – YD) of the CROPGRO-soybean model as a function of different groupings of experiments.

Despite few sets of genetic coefficients in the individual sowings group had the same or slightly lower RRMSE, almost all the datasets showed higher errors (Figure 4). Among all the developmental stages, the highest errors were found when the individual experiments 6 and 12 were used to calibrate the model, indicating model inability to properly simulate the developmental stages for late (February) and early (September) sowing dates, respectively.

The calibration/validation using all the data together class, seemed highly reliable compared to other groups to estimate the phenological stages (Figure 4). This group showed the lowest RRMSE's, with an average developmental stage RRMSE from 4.5% to 10.9, compared to the 8.4 to 22.2%, 8.5 to 10% and 7.9 to 8.8 in Individual sowings, season/year per location, experimental site, respectively. For the final leaf number (FLN), the RRMSE varied from 14.7 to 18.7%, 14.1 to 19.4%, 15.1 to 19.4% and 15% for individual sowings, season/year per location, experimental site and all data together, respectively. The model also showed limitations to simulate the FLN in early (September) and late (February) sowing dates. For example, in the earliest sowing date experiment, the average observed FNF (29 leaves) was 38% higher than the simulated FNF

(21 leaves). On the other hand, in the latest sowing date (February), the average observed FNF (9 leaves) was 44% lower than the simulated value (13 leaves). Usually, the early sown soybean had higher FNF due to a longer vegetative phase, which also contributed to a higher observed LAI.

For the LAI the RRMSE varied from 35 to 48% among the individual sowings. As generally observed in the other variables, the RRMSE also decreased as the grouping level increased, decreasing to 35% when the all data together group was used. These errors can be partly explained by the model inability to correctly simulate the LAI variability (observed and simulated LAI varied from 2.3 to 8.7 and 0.94 to 6.92, respectively). The higher observed LAI occurred in a early sowing dates (8.7), but the higher simulated LAI occurred in the optimum sowing date (6.92).

The relative errors in canopy height varied from 21 to 34%, 17 to 35%, 21 to 35% and 21% for the individual sowings, season/year per location, experimental site and all data together, respectively. The CROPGRO-soybean model usually underestimated canopy height, which could be partly explained by the longer and taller varieties cropped in Brazil, compared to the shorter cycle varieties in the USA, where the model was developed.

In the one-grain dry mass (OG) RRMSEs, the range was from 13 to 35%, 18 to 20%, 18 to 22% and 26% for individual sowings, season/year per location, experimental site and all data together, respectively. These errors were partly explained by the large observed one grain dry mass variability (from 0.11 to 0.24 grams) among all the different sowing dates.

The grain number per meter square ( $\text{grains.m}^{-2}$ ) RRMSE varied from 18 to 35%, 19 to 22%, 18 to 22% and 21% for individual sowings, season/year per location, experimental site and all data together, respectively. The grain yield RRMSE varied from 27 to 36%, 30%, 28 to 30% and 28%

for individual sowings, season/year per location, experimental sites and all data together, respectively.

Considering the phenological stages and the two growth parameters without missing measurements (final leaf number and canopy height), the all data together group showed an average RMSE of 11%. This error was the same found in the individual sowings, season/year per location, and experimental site groups that varied from 11 to 23%, 11 to 14 and 11 to 14%, respectively.

Despite some individual sowings group showed lower RRMSE values than the obtained in other groups, it is important to highlight that this class also showed the highest RMSEs (28.4, 48, and 36% to simulate R1, LAI and grain yield, respectively). Therefore, considering the errors that an individual sowing could lead, it is too risky to use only one experiment to calibrate the CROPGRO-soybean model. Moreover, increasing the grouping level from individual sowings to season/year per location (early, optimum and late sowing dates), decreased the phenology RRMSE range from 4.1 to 28.7% to from 4.4 to 12.6%. If I drew a curve between grouping level and the RRMSE' the resulting curve begins to be asymptotic on season/year per location group. The results of this manuscript are very specific for soybean and not necessary to extrapolated for other crops.

#### **4. DISCUSSION**

This study aims to found answers capable to enlarge and facilitate crop model calibration/validation, and to reduce risks, costs and time related to field experiments. Despite crop models have been available for more than 3 decades of existence, developing countries rarely manage to take full advantage of them to improve management decisions. Then, optimizing the minimum number of field experiments to calibrate/validate the models and to take full advantage

of the models, will allow better use of available resources increasing the impact on agricultural research.

As found by Thorp et al (2007), in this study as the grouping level increased (from individual sowings to all data together) the average RRMSE's also decreased. In this study, the phenological RRMSE's range decreased from 4.1 to 28.7% to 4.5 to 10.9% from individual sowings and all data together. The model predicted the growth variables with higher RRMSE's (from 15 to 50%) compared to the phenological stages (around 10%).

The optimum number of experiments found in this study was obtained from season/year per location group. The use of three sowing dates (early, optimum and late) allow us to cover the entire soybean sowing window, which will increasing the simulations accuracy under management changes.

## **5. CONCLUSIONS**

The results showed that in general, the use of all data together group to estimate the development and growth coefficients resulted in the lowest RRMSE's among all four groups. However, as the experiment number increased it also increased the costs and time. Then, in order to increase the research resources efficiency, as well as to achieve a reliable cultivar calibration/validation, we can conclude that researchers should use the season/year per location group (three experiments). This strategy will allow modelers to capture the genetic coefficient of a soybean variety under the entire sowing window avoiding the high uncertainties and costs from individual experiment and all data together, respectively.

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Table S1 – Set of genetic coefficients estimated using each dataset used in the four different grouping levels during the calibration/validation procedures in this study.

Classes	Development genetic coefficients					Growth genetic coefficients					
	EM-FL	FL-SH	FL-SD	SD-PM	FL-LF	LFMAX	SLAVR	SIZLF	WPSD	PODUR	SFDUR
<b>Individual Sowings</b>											
Exp.1	24.1	5.3	14	41.4	28	1.030	400	240	0.18	10	23
Exp.2	24.3	5.3	14	41.0	26	1.030	400	240	0.18	10	23
Exp.3	26.0	3.6	11	39.7	36	1.400	400	240	0.12	10	23
Exp.4	23.5	4.7	16	35.7	30	1.400	315	221	0.22	10	23

Exp.5	25.9	4.3	11	35.7	22	0.820	345	201	0.14	10	23
Exp.6	28.3	8.8	20	26.3	28	1.200	400	200	0.24	10	23
Exp.7	26.6	5.8	13	39.7	28	1.200	365	260	0.12	10	23
Exp.8	25.0	3.7	14	39.2	30	1.300	375	281	0.18	10	23
Exp.9	26.1	6.2	11	36.0	26	0.900	345	201	0.12	10	23
Exp.10	26.3	7.0	17	30.8	36	1.400	400	290	0.21	10	18
Exp.11	24.3	4.1	12	35.8	18	0.900	350	240	0.14	14	18
Exp.12	17.2	5.5	12	37.3	28	1.170	340	240	0.11	14	18
Exp.13	26.4	5.7	15	33.9	8	0.820	400	170	0.19	14	23
Exp.14	28.5	3.1	12	40.3	8	1.400	320	270	0.21	3	23
Exp.15	23.4	5.6	11	41.6	16	1.060	300	180	0.21	3	25
Exp.16	24.3	4.7	10	38.2	26	1.130	330	200	0.19	3	23
Exp.17	23.3	8.9	16	36.9	7	1.300	320	200	0.18	3	23
Exp.18	21.4	12.9	16	37.4	30	0.820	310	200	0.17	7	23
Exp.19	23.4	7.5	16	39.8	16	0.820	300	200	0.17	7	18
Exp.20	27.0	6.9	16	35.6	36	0.820	400	150	0.18	6	18
Exp.21	26.5	4.2	11	35.6	30	0.820	400	150	0.13	11	15
<b>Season/year per location</b>											
Field 1	23.9	5.7	14	40.6	26	1030	300	200	0.18	10	23
Field 2	25.1	3.9	12	37.9	36	1300	315	180	0.15	10	23
Field 3	26.7	7.2	14	37.4	36	1100	385	180	0.11	7	17
Field 4	24.0	4.3	13	36.3	10	820	400	180	0.13	6	13
Field 5	23.5	8.2	13	38.9	30	820	315	200	0.15	14	22
<b>Experimental site</b>											
Station 1	24.7	6.5	14	36.2	30	820	300	250	0.13	5	13
Station 2	23.5	8.2	13	38.9	30	820	315	200	0.15	14	22
<b>All data together</b>											
Program	24.8	6.0	13.4	37.0	26	0.93	345	221	0.2	10	26

Table S2 – Relative root mean square errors (%) resulted from each set of genetic coefficients used (Table S1) during the CROPGRO-soybean model validation procedure.

Groups	Development genetic coefficients				Growth genetic coefficients						
	EM-FL	FL-SH	FL-SD	SD-PM	Final Leaf num.	LAI	C. H.	One Grain	Grains/m <sup>2</sup>	Grain yield	Averag. RMSE
<b>Individual sowings</b>											
Exp. 1	8.0	9.5	10.9	6.1	14.7	N	25	N	N	N	11.8
Exp. 2	7.8	9.3	11.0	5.5	14.7	N	25	N	N	N	11.7
Exp. 3	9.1	9.9	12.0	4.8	14.7	N	24	22.2	N	N	13.2
Exp. 4	9.3	11.6	10.9	4.4	14.7	N	26	30.5	N	N	14.6
Exp. 5	8.3	9.1	12.5	5.5	15.3	N	27	18.0	N	N	13.1

Exp.6	15.2	19.6	24.9	6.7	18.1	N	27	17.6	N	N	18.2*
Exp.7	10.3	9.4	11.3	6.6	15.3	N	25	20.6	N	N	13.5*
Exp.8	7.9	11.1	10.8	5.1	14.7	N	25	18.7	N	N	12.8*
Exp.9	8.9	9.2	12.2	5.1	15.3	N	26	18.8	N	N	13.0*
Exp.10	9.8	11.0	15.5	5.1	15.8	48	26	32.2	27	35	21.4
Exp.11	7.7	11.5	12.1	5.1	15.3	37	26	17.5	21	30	17.5
Exp.12	28.7	24.7	24.9	10.6	17.0	37	27	17.2	34	31	24.9
Exp.13	9.0	9.0	12.4	5.1	15.8	39	34	16.7	24	33	18.8
Exp.14	9.5	9.2	12.8	5.0	16.4	44	27	13.0	24	34	18.5
Exp.15	9.3	10.1	15.9	4.6	18.1	39	24	35.3	19	27	19.3
Exp.16	7.5	10.4	15.3	5.7	18.7	35	24	30.4	24	29	19.1
Exp.17	9.3	9.2	10.9	4.6	15.3	40	22	20.8	35	36	19.2
Exp.18	14.8	14.3	11.2	4.1	15.3	35	22	32.8	21	30	19.2
Exp.19	9.3	8.5	10.8	6.0	15.3	N	22	20.6	18	27	14.6*
Exp.20	10.9	12.0	14.4	6.7	15.8	35	21	19.0	22	30	18.0
Exp.21	9.4	8.8	12.1	5.5	15.3	35	21	19.2	25	33	17.6
<b>Season/year per location</b>											
Field 1	8.2	9.3	10.9	5.4	14.3	N	22	N	N	N	11.3*
Field 2	7.5	10.8	12.1	4.6	14.3	N	21	17.6	N	N	12.1*
Field 3	10.1	12.2	11.7	5.9	14.7	N	17	17.6	N	N	12.4*
Field 4	8.3	11.5	12.1	4.9	14.1	44	23	19.3	19	30	17.7
Field 5	9.3	8.8	12.6	4.4	19.4	35	35	19.6	22	30	18.6
<b>Experimental sites</b>											
Station 1	7.6	8.6	10.8	4.5	15.1	35	21	17.6	18	28	15.8
Station 2	9.3	8.8	12.6	4.4	19.4	35	35	19.6	22	30	18.6
<b>All data together</b>											
Program	7.5	8.3	10.9	4.5	15.3	35	21	26.0	21	28	16.9

\*Averages without grains.m<sup>-2</sup> and yield.

Table S3 – Layer by layer information of all soils used in this study.

Location	Layer	Depth (cm)	Silt (%)	Sand (%)	Clay (%)
Santa Maria	A	15	42	35	23
	A	30	22	53	25
	B	55	16	37	47
	B	70	23	27	50
	B	87	33	13	54
	C	120	35	5	60
Júlio de Castilhos	A	13	11	54	35
	AA	35	8	70	22
	AAA	55	8	66	26
	B	100	8	65	27
	BB	300	8	60	32
	A	17	22	9	69
Frederico Westphalen	AAA	40	22	11	67
	B	58	19	11	70
	BB	120	14	9	77

	<b>BB</b>	<b>180</b>	<b>12</b>	<b>6</b>	<b>82</b>
	<b>BB</b>	<b>440</b>	<b>13</b>	<b>8</b>	<b>79</b>
	<b>BBB</b>	<b>530</b>	<b>18</b>	<b>8</b>	<b>74</b>
	<b>A</b>	<b>23</b>	<b>36</b>	<b>55</b>	<b>19</b>
<b>Pelotas</b>	<b>AA</b>	<b>40</b>	<b>36</b>	<b>50</b>	<b>14</b>
	<b>B</b>	<b>80</b>	<b>28</b>	<b>30</b>	<b>42</b>
	<b>BB</b>	<b>110</b>	<b>31</b>	<b>35</b>	<b>34</b>
	<b>A</b>	<b>20</b>	<b>43</b>	<b>36</b>	<b>21</b>
<b>Restinga Seca</b>	<b>A</b>	<b>40</b>	<b>28</b>	<b>57</b>	<b>15</b>
	<b>AB</b>	<b>55</b>	<b>33</b>	<b>44</b>	<b>23</b>
	<b>B</b>	<b>75</b>	<b>63</b>	<b>15</b>	<b>22</b>
	<b>C</b>	<b>115</b>	<b>72</b>	<b>18</b>	<b>10</b>
	<b>A</b>	<b>17</b>	<b>62</b>	<b>20</b>	<b>18</b>
<b>Itaqui</b>	<b>A</b>	<b>35</b>	<b>38</b>	<b>37</b>	<b>25</b>
	<b>B</b>	<b>65</b>	<b>26</b>	<b>21</b>	<b>53</b>
	<b>A</b>	<b>10</b>	<b>21</b>	<b>10</b>	<b>69</b>
	<b>AAA</b>	<b>30</b>	<b>21</b>	<b>9</b>	<b>70</b>
	<b>B</b>	<b>51</b>	<b>13</b>	<b>7</b>	<b>80</b>
<b>Água Santa</b>	<b>B</b>	<b>95</b>	<b>13</b>	<b>4</b>	<b>83</b>
	<b>BB</b>	<b>133</b>	<b>14</b>	<b>8</b>	<b>78</b>
	<b>BB</b>	<b>182</b>	<b>16</b>	<b>9</b>	<b>75</b>
	<b>BB</b>	<b>222</b>	<b>18</b>	<b>9</b>	<b>73</b>
	<b>BB</b>	<b>280</b>	<b>25</b>	<b>13</b>	<b>62</b>
	<b>C</b>	<b>320</b>	<b>29</b>	<b>29</b>	<b>42</b>
	<b>C</b>	<b>380</b>	<b>32</b>	<b>33</b>	<b>35</b>
	<b>A</b>	<b>13</b>	<b>9</b>	<b>45</b>	<b>46</b>
<b>Tupanciretã</b>	<b>AA</b>	<b>35</b>	<b>8</b>	<b>70</b>	<b>22</b>
	<b>AAA</b>	<b>55</b>	<b>8</b>	<b>66</b>	<b>26</b>
	<b>B</b>	<b>100</b>	<b>8</b>	<b>65</b>	<b>27</b>
	<b>BB</b>	<b>300</b>	<b>8</b>	<b>60</b>	<b>32</b>

## 7 DISCUSSÃO

Modelos agrícolas são ferramentas que podem trazer inúmeros benefícios para a agricultura, principalmente em países em desenvolvimento, onde a economia geralmente possui forte dependência do setor agrícola. Entre as principais dificuldades para aumento no número de usuários, são os processos de calibração e de validação do modelo e o alto custo financeiro para a condução de experimentos necessários para calibrar e validar, dificuldades enfrentadas principalmente por países em desenvolvimento, visto que existe um número mais expressivo de usuários e de pesquisa em modelagem em países desenvolvidos.

Diminuir as incertezas envolvidas nos processos de calibração e validação pode facilitar e otimizar a utilização de modelos agrícolas, e conseqüentemente torná-los mais acessíveis para extensionistas agrícolas de setores governamentais e privados. Como exemplos da utilização de modelos agrícolas na busca de um melhor entendimento sobre as interações (genótipo X ambiente X manejo) das culturas, visando maior eficiência no manejo e planejamento agrícola, estão os

modelos SimulArroz ([www.ufsm.br/simularroz](http://www.ufsm.br/simularroz)), o Simanihot ([www.ufsm.br/simanihot](http://www.ufsm.br/simanihot)) e PhenoGlad ([www.ufsm.br/phenoglad](http://www.ufsm.br/phenoglad)).

O Modelo CROPGRO-soybean é um dos modelos mais utilizados por pesquisadores para pesquisa em Soja, porém, aqui no Brasil tem seu uso bastante restrito e tímido. O grande número de parâmetros iniciais que esse modelo necessita, é um dos principais obstáculos quando é tentado utilizá-lo com dados obtidos em experimentos de campo. Isso, somado às restrições financeiras que encurtam a cada ano o orçamento para pesquisa, aumenta a necessidade de um método capaz de utilizar com maior eficiência os dados obtidos em um número reduzido de experimentos.

No primeiro capítulo desta tese, o método cross-validation LOO, capaz de utilizar todos os conjuntos de experimentos nos processos de calibração e validação, foi comparado com o método de partição em dois grupos para calibrar e validar o cultivar NA 5909. Pelo método de partição em dois grupos, um conjunto de experimentos foi dividido em duas partes, uma para calibrar e a outra para validar o modelo. Fatos como o encurtamento no período de mercado de uma cultivar, o alto número de cultivares lançadas a cada ano e restrições no orçamento para a condução de múltiplos experimentos, faz com que geralmente exista um número reduzido de experimentos. Assim, a divisão de um conjunto pequeno de experimentos em duas partes, pode afetar negativamente a calibração e validação do modelo, resultando em uma calibração tendenciosa, de acordo com a divisão adotada. Assim, métodos que possam trazer maior robustez aos processos de calibração e validação são sempre vindos, pois melhoram a precisão e diminuem o número necessário de experimentos para executar o mesmo processo.

O método cross-validation, tem como principal característica, permitir a utilização de todos os experimentos, tanto na calibração quanto na validação, foi comparado ao método de partição em dois grupos. Pelo método de partição em dois grupos, os 21 experimentos foram divididos em duas partes, sendo a primeira para calibração e a segunda para validação. O método de calibração/validação cross-validation reduziu o erro médio quadrático das simulações dos estádios fenológicos de 2.6, 4.6, 4.8, 7.3, 10.2 para 1.1, 4.1, 4.1, 6.2, 6.3 dias para emergência, R1, R3, R5 e R7, respectivamente. Já para os componentes de rendimento, o método cross-validation reduziu o erro médio quadrático de 677 e 551 para 347 e 447 grãos.m<sup>-2</sup> e kg.ha<sup>-1</sup>, respectivamente. Foi observado baixa variabilidade (estabilidade dos coeficientes genéticos) nos valores estimados na maioria dos 21 experimentos. Isso significa que os coeficientes genéticos de cultivar NA 5909,

poderiam ter sido obtidos, a partir de um número inferior de experimentos e datas de semeadura, economia que poderia ser revertida em novos experimentos ou novas cultivares por exemplo.

Mesmo considerando a ampla faixa de datas de semeadura (Setembro á Fevereiro) e de condições ambientais (clima, solos e diferentes anos agrícolas), o modelo CROPGRO-soybean, se mostrou robusto nas previsões dos estágios fenológicos, acúmulo de biomassa e produtividade. Na calibração e validação dos coeficientes genéticos específicos de uma cultivar, o método cross-validation deveria ser utilizado sempre que possível, pois, ao permitir a utilização total de experimentos durante a calibração/validação (evita a divisão em duas partes), permite também a redução de experimentos necessários, e conseqüentemente os custos, sem prejudicar o desempenho do modelo CROPGRO-soybean. Ou seja, se pelo método partição em dois grupos, com 10 experimentos, utilizo 6 para calibrar e 4 para validar. Já com o método cross-validation, com apenas 6 experimentos, o modelo é calibrado e validado com os 6, garantindo uma menor tendenciosidade durante os processos.

Os resultados do primeiro capítulo, também sugerem que ao eliminar a necessidade da divisão do conjunto de experimentos, o método cross-validation leave-one-out, pode reduzir o número de experimentos necessários para calibrar e validar o modelo CROPGRO-soybean. O processo de calibração e validação geralmente utiliza vários experimentos ou um número mais restrito. Calibrar e validar um modelo utilizando poucos experimentos, pode incrementar as incertezas, já um conjunto maior, apresenta custos elevados e inviáveis. Assim, o objetivo principal do segundo capítulo desta tese, foi quantificar as incertezas envolvidas nos processos de calibração e validação utilizando diferentes números de experimentos, e estimar o número mínimo de experimentos para uma calibração confiável do modelo CROPGRO-soybean.

O estudo conduzido com o total de 21 experimentos (cultivar BMX Potência RR), semeada em 8 locais diferentes no Estado do Rio Grande do Sul, durante 4 anos agrícolas (2010/2011 a 2013/2014), permitiu obter uma grande quantidade de dados representativos de diferentes condições ambientais. Assim, essa grande quantidade de dados, possibilitou a realização de uma análise por agrupamentos. Os 21 experimentos agrupados em 4 grupos diferentes (semeaduras individuais), ano agrícola por local (mais de uma data de semeadura no mesmo ano agrícola e local), local experimental (todos os experimentos conduzidos no mesmo local) e todos os 21 experimentos disponíveis juntos, resultaram em 28 diferentes combinações distribuídas nos 4

grupos. Em todas as 4 classes, os processos de calibração e validação foram conduzidos utilizando o método cross-validation leave-one-out.

Em geral, a variabilidade dos coeficientes genéticos, diminuiu conforme o número de experimentos utilizados na calibração aumentou. A variabilidade dos RRMSEs também diminuiu ao ser aumentado o nível do agrupamento, porém, o maior decréscimo ocorre com o avanço do grupo de sementes individuais (primeiro grupo) para a ano agrícola por local (segundo grupo). Calibrar o modelo CROPGRO-soybean, utilizando apenas um dos experimentos do grupo 1, pode levar a erros nas simulações de 28.4, 48 e 36% para estimar a data do estágio R1, o IAF e a produtividade, respectivamente. A mudança do primeiro grupo para o segundo, apresentou um leve acréscimo no erro mínimo, mas reduziu a amplitude dos erros relativos (RRMES's) de 4.1 a 28.7 para 4.4 a 12.6% nas simulações dos estádios fenológicos (R1, R3, R5 e R7), ou seja, os erros decresceram mais do que duas vezes (28.7% na fenologia). Esse primeiro resultado eleva a necessidade de aplicar o método cross-validation na calibração/validação nos casos em que o pesquisador possui um número pequeno de experimentos.

Ao aumentar o nível de agrupamento (grupos 3 e 4), o decréscimo nas variabilidades (coeficientes genéticos e dos erros) também foi observado. Porém, os decréscimos foram sutis, ou seja, não justificam triplicar ou setuplicar o número de experimentos. Em outras palavras, desenhando uma curva partindo do grupo 1 até o grupo 4, é como se a curva se tornasse assintótica, não oferecendo benefícios significativos.

## 8 CONCLUSÃO

Os coeficientes estimados a partir do método cross-validation leave-one-out, apresentaram melhor desempenho quando comparados ao método de partição em dois grupos durante a calibração e validação do modelo CROPGRO-soybean. Para aumentar o desempenho e a eficiência do uso dos experimentos disponíveis nos processos de calibração e validação, o método cross-validation deve ser usado sempre que possível.

Em geral, quanto maior o nível de agrupamento (mais experimentos), menores os valores dos erros relativos (RRMSEs) durante as simulações do modelo CROPGRO-soybean. Porém, o número mínimo de experimentos necessários para alcançar uma calibração e validação de

qualidade, são 3 experimentos grupo 2. Essa estratégia permite compreender as interações (genótipo x ambiente x manejo) dentro de uma ampla faixa de semeadura e evita as incertezas do grupo 1 e os altos custos que conjuntos maiores de experimentos demandam.

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## 10 APÊNDICE

Passo-á-passo simplificado, das etapas necessárias para a utilização do modelo CROPGRO-soybean.

Passo 1 -> Criar o arquivo \*.SBA – responsável pelos dados observados nos experimentos (finais como as datas fenológicas, número final de nós, produtividade e outros). Na pasta Soybean, existem vários modelos de arquivos \*.SBA, que podem ser utilizados como modelo de partida.

```

! File last edited on day 08/27/2013 at 4:14:32 PM
!
@TRNO PDAT EDAT ADAT PD1T PDFT MDAT
1 344 351 030 040 054 097
2 008 015 050 058 070 114
3 267 275 334 345 005 062
4 323 330 020 031 051 091
5 028 034 069 074 083 127
6 266 277 324 340 363 047
7 308 314 001 011 026 076
8 337 343 025 035 048 095
9 037 042 079 088 099 144
10 270 278 327 338 360 040
11 319 324 007 018 030 080
12 050 055 090 097 107 156
13 322 328 019 026 039 084
14 327 333 015 023 038 072
15 314 320 008 017 033 085
16 318 323 005 020 030 073
17 289 295 348 013 -99 077
18 328 333 020 048 -99 093
19 345 351 035 051 -99 105
20 337 344 024 039 060 094
21 321 326 020 029 040 086

```

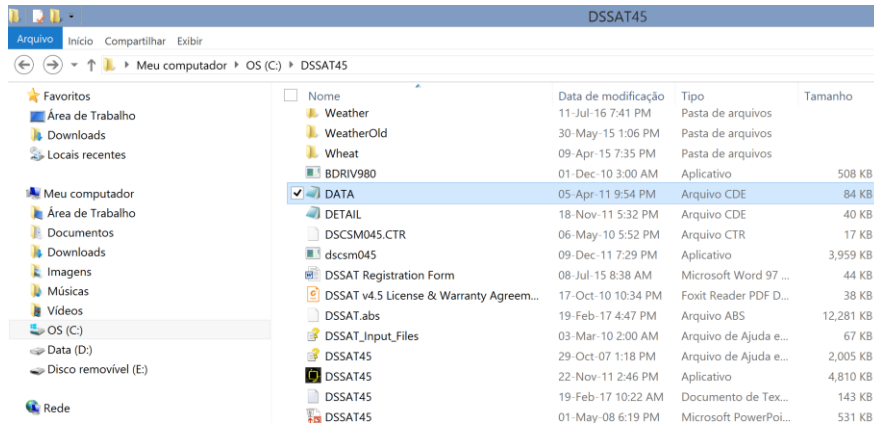
Passo 2 -> Criar o arquivo \*.SBT – responsável pela alocação de dados que serão comparados de forma continua durante as simulações, como evolução de número de nós, evolução da massa de grãos, etc. Na mesma pasta do Passo 1 (Soybean), também existem arquivos \*.SBT experimentos que podem ser utilizados como ponto de partida.

```

! File last edited on day 08/27/2003 at 4:10:58 PM
!
@TRNO DATE L#SD LAID P#AD SHAD GHAD LHAD CWAD PHAD SHAD RWAD G#AD SH#D SLAD GWGD HIAD HIPD
1 88165 2.0 0.51 0.0 28.5 0.0 174.2 202.8 0.0 0.0 -99 0.0 -99 290 -99 -99 -99
1 88172 3.5 0.86 0.0 133.8 0.0 330.4 464.1 0.0 0.0 -99 0.0 -99 262 -99 -99 -99
1 88179 5.2 2.35 0.0 440.5 0.0 809.2 1250 0.0 0.0 -99 0.0 -99 291 -99 -99 -99
1 88187 7.2 2.66 0.0 766.6 0.0 1065 1832 0.0 0.0 -99 0.0 -99 250 -99 -99 -99
1 88193 9.2 4.82 0.0 1355 0.0 1490 2845 0.0 0.0 -99 0.0 -99 323 -99 -99 -99
1 88200 11.2 5.31 0.0 1679 0.0 1576 3255 0.0 0.0 -99 0.0 -99 337 -99 -99 -99
1 88207 13.8 6.03 0.0 2337 0.0 2027 4364 0.0 0.0 -99 0.0 -99 298 -99 -99 -99
1 88214 15.2 5.66 257.4 2654 0.0 1809 4491 0.0 0.0 -99 0.0 -99 313 -99 -99 -99
1 88221 18.8 7.65 969.8 4711 2.5 2755 7749 50.2 47.7 -99 97.5 5.0 278 2.5 0.000 0.006
1 88228 20.2 6.24 1501 4618 178.3 2237 7779 788.2 609.9 -99 1659 22.6 279 9.8 0.023 0.101
1 88235 21.5 6.41 1549 5010 668.8 2512 9676 2132 1463 -99 1597 31.4 255 41.8 0.069 0.220
1 88242 23.5 4.94 1305 4625 1527 2008 9678 3041 1514 -99 2574 50.2 246 58.7 0.158 0.314
1 88250 24.0 4.18 1310 4447 2679 1854 10641 4338 1659 -99 3020 61.7 225 89.1 0.252 0.408
1 88256 22.5 3.55 1234 4204 3148 1416 10316 4692 1545 -99 2687 67.1 251 123.0 0.305 0.455
1 88263 23.2 1.72 1089 3203 3558 590.7 8666 4866 1308 -99 2575 73.1 291 137.8 0.411 0.562
1 88270 23.2 0.00 1253 3010 4723 0.0 9265 6222 1499 -99 2976 75.9 -99 158.3 0.510 0.672
1 88277 23.0 0.00 1127 2671 4151 0.0 8091 5369 1218 -99 2597 77.3 -99 161.0 0.513 0.664
1 88289 -99 -99 -99 -99 3802 -99 -99 -99 -99 2658 -99 -99 143.0 -99 -99

```

Na pasta inicial do DSSAT, o arquivo de texto DATA, contém informações sobre o significado da maioria das siglas utilizadas durante a confecção dos arquivos iniciais.



Passo 3 -> A criação do arquivo SBX, o qual será o responsável pelos detalhes do manejo de cada experimento que será simulado. Ao abrir o programa DSSAT, na aba esquerda (FERRAMENTAS), o sub-programa Crop Management Data irá auxiliar na criação desse arquivo.

**General Information-**

**File Type** Experimental

**Experiment Name** \_\_\_\_\_

**Experiment Identifier (file name)** \_\_\_\_\_

**Institute Code** \_\_\_\_\_

**Site Code** \_\_\_\_\_

**Year** \_\_\_\_\_

**Experiment Number** \_\_\_\_\_

**Crop** \_\_\_\_\_

**General Information**

**People** \_\_\_\_\_

**Address** \_\_\_\_\_

**Site** \_\_\_\_\_

**Plot Information**

**Gross Plot Area per rep, m2** \_\_\_\_\_

**Rows per Plot** \_\_\_\_\_

**Plot Length, m** \_\_\_\_\_

**Plots Relative to Drains, degrees** \_\_\_\_\_

**Plot Spacing, cm** \_\_\_\_\_

**Plot Layout** \_\_\_\_\_

**Harvest Information**

**Harvest Area, m-2** \_\_\_\_\_

**Harvest Row Number** \_\_\_\_\_

**Harvest Row Length, m** \_\_\_\_\_

**Harvest Method** \_\_\_\_\_

**Additional Information** **Next >**

Passo 4 -> Será necessária a seleção de uma estação meteorológica para cada experimento, ou a mesma para vários experimentos de acordo com a disponibilidade e proximidade.

Passo 5 -> Na pasta Weather, existem várias estações meteorológicas já utilizadas no modelo, e podem servir como modelo de como os dados devem ser organizados. Uma opção mais fácil é a utilização do subprograma Weather Data (Localizado na aba esquerda (FERRAMENTAS)). OBS – Certifique-se que as coordenadas geográficas estejam corretas, no arquivo da estação meteorológica, pois o modelo utiliza essas coordenadas para estimar o fotoperíodo, e não as inseridas durante a criação do arquivo SBX.

```

*WEATHER DATA : RSSA
@ INSI  LAT   LONG  ELEV  TAV  AMP  REFHT  WNDHT
RSSA  -29.700 -53.700 113  12.8  13.3 -99.0 -99.0
@DATE  SRAD  TMAX  TMIN  RAIN  DEWP  WIND  PAR  EVAP  RHUM
14001  15.0  28.1  17.8  3.8
14002  15.7  27.3  19.2  1.4
14003  5.4   20.8  14.7  51.6
14004  19.1  22.7  13.9  2.0
14005  26.7  27.8  13.8  0.0
14006  28.0  29.8  15.0  0.0
14007  28.9  29.0  16.3  1.4
14008  18.6  26.7  15.5  6.4
14009  24.3  28.2  16.8  2.6
14010  28.3  29.2  16.2  19.0
14011  12.8  26.3  15.0  40.0
14012  7.6   20.8  17.1  27.6
14013  19.0  25.4  16.6  0.2
14014  22.0  25.3  16.2  0.0
14015  13.2  23.3  14.8  1.8
14016  27.3  26.8  13.2  0.2
14017  32.4  29.3  15.7  0.0
14018  26.2  28.8  15.8  0.0

```

Passo 6 -> Um arquivo com informações detalhadas do perfil de solos do local do experimento, também é necessário na etapa da criação do arquivo do experimento (da mesma forma que o arquivo da estação meteorológica). Na pasta Soil, existem alguns arquivos de solos que podem ser utilizados como exemplo (base) durante a confecção. O significados das siglas são encontrados nos arquivos DATA e SOIL, localizados na pasta principal DSSAT.

```

BR - Bloco de notas
Arquivo Editar Formatar Exibir Ajuda
*BRPI020004 UFSMS L 120 ARGISSOL BRUNO, SOIL AF001
@SITE COUNTRY LAT LONG SCS Family
StaMaria Brazil -29.600 -53.800 ARGISSOLO BRUNO
@ SCOM SALB SLU1 SLDR SLRO SLNF SLPF SMHB SMPX SMKE
BN 0.13 6.00 0.30 76.00 1.00 0.98 SA001 SA001 SA001
@ SLB SLMH SLLL SDUL SSAT SRGF SSKS SBDM SLOC SLCL SLSI SLCF SLNI SLHW SLHB SCEC SADC
15 A 0.183 0.338 0.480 1.000 0.68 1.38 2.50 23.00 42.00 -99.0 -99.0 6.30 -99.0 12.6 -99.0
30 A 0.193 0.335 0.480 0.638 0.45 1.40 0.83 25.00 22.00 -99.0 -99.0 6.00 -99.0 12.0 -99.0
55 B 0.265 0.400 0.510 0.427 0.14 1.28 0.72 47.00 16.00 -99.0 -99.0 5.70 -99.0 12.0 -99.0
70 B 0.274 0.408 0.530 0.286 0.17 1.25 0.51 50.00 23.00 -99.0 -99.0 5.50 -99.0 12.0 -99.0
87 B 0.285 0.418 0.540 0.208 0.22 1.21 0.32 54.00 33.00 -99.0 -99.0 5.50 -99.0 12.0 -99.0
120 C 0.300 0.432 0.550 0.126 0.26 1.19 0.19 60.00 35.00 -99.0 -99.0 5.50 -99.0 12.0 -99.0

*BRPI020005 UFSMS L 115 ARGISSOL BRUNO, SOIL AF001
@SITE COUNTRY LAT LONG SCS Family
Restinga Brazil -29.7 -53.4 ARGISSOLO BRUNO
@ SCOM SALB SLU1 SLDR SLRO SLNF SLPF SMHB SMPX SMKE
BN 0.13 6.00 0.40 78.00 1.00 0.97 SA001 SA001 SA001
@ SLB SLMH SLLL SDUL SSAT SRGF SSKS SBDM SLOC SLCL SLSI SLCF SLNI SLHW SLHB SCEC SADC
20 A 0.176 0.312 0.470 1.000 0.82 1.39 2.40 21.00 43.00 -99.0 -99.0 5.20 -99.0 12.6 -99.0
40 A 0.148 0.281 0.440 0.549 1.37 1.48 0.86 15.00 28.00 -99.0 -99.0 5.20 -99.0 12.0 -99.0
55 AB 0.184 0.321 0.470 0.387 0.61 1.39 0.69 23.00 33.00 -99.0 -99.0 6.00 -99.0 11.8 -99.0
75 B 0.180 0.316 0.490 0.273 1.02 1.35 0.40 22.00 63.00 -99.0 -99.0 6.00 -99.0 11.8 -99.0
115 C 0.120 0.248 0.450 0.149 3.12 1.47 0.32 10.00 72.00 -99.0 -99.0 6.00 -99.0 11.8 -99.0
    
```

Passo 7 -> No quadro 1, é possível encontrar os coeficientes genéticos que apresentaram os melhores desempenhos nas simulações das cultivares NA 5909 e BMX Potência, a partir dos 21 experimentos do projeto. Esses coeficientes devem ser inseridos como novas linhas (como no exemplo abaixo), no arquivo SBGRO045.CUL, localizado dentro da pasta Genotype.

```

!VAR# VRNAME..... ECO# CSDL PPSEN EM-FL FL-SH FL-SD SD-PM FL-LF LFMAX SLAVR SIZLF XFRT WTPSD SFDUR SDPDU PODUR
CF0001 BMXtu RSSM . SB0607 12.58 0.311 22.0 3.0 10.7 25.90 18.00 1.030 375. 180.0 1.00 0.18 23.0 2.05 10.0 78.0 .400 .200
CF0002 BMXen RSSM . SB0507 12.83 0.303 24.5 4.4 10.7 31.50 18.00 1.030 375. 180.0 1.00 0.18 23.0 2.05 10.0 78.0 .400 .200
CF0003 NS482 RSSM . SB0407 13.09 0.294 17.6 13.4 18.3 35.70 26.00 1.030 375. 180.0 1.00 0.19 23.0 2.20 10.0 77.0 .405 .205
CF0004 IAS 5 RSSM . SB0606 12.58 0.311 23.2 10.9 13.0 30.00 18.00 1.030 375. 180.0 1.00 0.18 23.0 2.05 10.0 78.0 .400 .200
CF0005 NA5909RSSM . SB0601 12.58 0.311 26.8 3.0 14.1 31.00 18.00 1.030 375. 180.0 1.00 0.18 23.0 2.05 10.0 78.0 .400 .200
CF0006 BMXPotRSSM . SB0605 12.58 0.311 25.1 4.6 12.7 38.20 18.00 1.030 375. 180.0 1.00 0.18 23.0 2.05 10.0 78.0 .400 .200
    
```

Quadro 1 – Coeficientes genéticos utilizados para executar as simulações no modelos CROPGRO-soybean de duas cultivares de soja.

Cultivar	EM-FL	FL-SH	FL-SD	SD-PM	FL-LF	LFMAX	SLAVR	SIZLF	WTPSD
NA 5909	23.4	5	11.6	34.1	26	1.000	355	220	0.17
BMX Potência	24.3	6	13.4	37.0	26	0.930	345	221	0.20

Passo 8 -> Após as simulações, são gerados inúmeros arquivos de saída (Outputs), com destaque para o OVERVIEW (apresenta informações gerais sobre as principais características de cada simulação) e o PLANTGRO (arquivo que apresenta a evolução diária detalhada, da maioria das variáveis simuladas pelo modelo, incluindo o balanço hídrico, estresses (excesso e déficit hídrico) e outros). Esses dois arquivos principais são apresentados nas 4 figuras abaixo.

OVERVIEW - Bloco de notas												
Arquivo Editar Formatar Exibir Ajuda												
CROP	:	Soybean	CULTIVAR	:	NA5909RSSM	ECOTYPE	:	SB0601				
STARTING DATE	:	JUL 18 2012										
PLANTING DATE	:	AUG 21 2012	PLANTS/m2	:	31.0	ROW SPACING	:	45.cm				
WEATHER	:	RSSA 2012										
SOIL	:	BRPI020004	TEXTURE	:	L	- ARGISSOL BRUNO, SOIL AF00						
SOIL INITIAL C	:	DEPTH:120cm	EXTR. H20:	164.6mm	NO3:	0.2kg/ha	NH4:	0.2kg/ha				
WATER BALANCE	:	RAINFED										
IRRIGATION	:	NOT IRRIGATED										
NITROGEN BAL.	:	SOIL-N, N-UPTAKE & DYNAMIC N-FIXATION SIMULATION										
N-FERTILIZER	:	NO N-FERTILIZER APPLIED										
RESIDUE/MANURE	:	INITIAL	:	0 kg/ha ;	0 kg/ha	IN	:	0 APPLICATIONS				
ENVIRONM. OPT.	:	DAYL=	0.00	SRAD=	0.00	TMAX=	0.00	TMIN=	0.00			
		RAIN=	0.00	CO2 =	0.00	DEW =	0.00	WIND=	0.00			
SIMULATION OPT	:	WATER	:Y	NITROGEN:	Y	N-FIX:	Y	PHOSPH	:N	PESTS	:N	
		PHOTO	:L	ET	:R	INFIL:	S	HYDROL	:R	SOM	:G	
		CO2	:W	NSWIT	:1	EVAP	:S	SOIL	:2			
MANAGEMENT OPT	:	PLANTING:	R	IRRIG	:N	FERT	:N	RESIDUE:	N	HARVEST:	M	
		WEATHER	:M	TILLAGE	:Y							
*SUMMARY OF SOIL AND GENETIC INPUT PARAMETERS												
SOIL DEPTH	LOWER	UPPER	SAT	EXTR	INIT	ROOT	BULK	pH	NO3	NH4	ORG	
DEPTH	LIMIT	LIMIT	SW	SW	SW	DIST	DENS				C	
cm	cm3/cm3	cm3/cm3	cm3/cm3	cm3/cm3	cm3/cm3		g/cm3		ugN/g	ugN/g	%	
0-	5	0.183	0.338	0.480	0.155	0.338	1.00	1.38	6.30	0.01	0.01	2.50
5-	15	0.183	0.338	0.480	0.155	0.338	1.00	1.38	6.30	0.01	0.01	2.50
15-	30	0.193	0.335	0.480	0.142	0.335	0.64	1.40	6.00	0.01	0.01	0.83
30-	42	0.265	0.400	0.510	0.135	0.400	0.43	1.28	5.70	0.01	0.01	0.72
42-	55	0.265	0.400	0.510	0.135	0.400	0.43	1.28	5.70	0.01	0.01	0.72
55-	70	0.274	0.408	0.530	0.134	0.408	0.29	1.25	5.50	0.01	0.01	0.51
70-	78	0.285	0.418	0.540	0.133	0.418	0.21	1.21	5.50	0.01	0.01	0.32
78-	87	0.285	0.418	0.540	0.133	0.418	0.21	1.21	5.50	0.01	0.01	0.32
87-	103	0.300	0.432	0.550	0.132	0.432	0.13	1.19	5.50	0.01	0.01	0.19
103-	120	0.300	0.432	0.550	0.132	0.432	0.13	1.19	5.50	0.01	0.01	0.19

OVERVIEW - Bloco de notas												
Arquivo Editar Formatar Exibir Ajuda												
TOT-120	31.1	47.6	62.4	16.5	47.6	<--cm	-	kg/ha-->	0.2	0.2	115826	
SOIL ALBEDO	:	0.13		EVAPORATION LIMIT	:	6.00		MIN. FACTOR	:	1.00		
RUNOFF CURVE #	:	76.00		DRAINAGE RATE	:	0.30		FERT. FACTOR	:	0.98		
Soybean CULTIVAR :CF0005-NA5909RSSM ECOTYPE :SB0601												
CSDVAR :12.58 PPSEN : 0.31 EMG-FLW:24.30 FLW-FSD:11.70 FSD-PHM : 34.40												
WTPSD :0.170 SDPVR : 3.05 SDFDUR :25.00 PODDUR : 8.00 XFRUIT : 1.00												
THRESH : 77.0 SDPRO :0.400 SDLIP : 0.200												
*SIMULATED CROP AND SOIL STATUS AT MAIN DEVELOPMENT STAGES												
RUN NO.	1	Sim1/2000										
DATE	CROP AGE	GROWTH STAGE	BIOMASS kg/ha	LAI	LEAF NUM	CROP N kg/ha	%	STRESS H2O	N	STRESS P1	P2	RSTG
18 JUL	0	Start Sim	0	0.00	0.0	0	0.0	0.00	0.00	0.00	0.00	0
21 AUG	0	Sowing	0	0.00	0.0	0	0.0	0.00	0.00	0.00	0.00	0
27 AUG	6	Emergence	14	0.02	0.0	1	5.1	0.00	0.00	0.00	0.00	0
27 AUG	6	End Juven.	14	0.02	0.0	1	5.1	0.00	0.00	0.00	0.00	0
7 SEP	17	Unifoliate	39	0.09	1.1	2	5.1	0.00	0.00	0.00	0.00	0
7 SEP	17	Flower Ind	39	0.09	1.1	2	5.1	0.00	0.00	0.00	0.00	0
15 OCT	55	First Flwr	945	2.00	7.7	34	3.6	0.00	0.02	0.00	0.00	1
24 OCT	64	First Pod	1827	3.10	9.6	66	3.6	0.00	0.00	0.00	0.00	3
6 NOV	77	First Seed	3489	4.10	12.5	116	3.3	0.00	0.00	0.00	0.00	5
28 NOV	99	End Msnode	6132	3.90	16.9	197	3.2	0.11	0.00	0.00	0.00	5
29 NOV	100	End Pod	6187	3.87	16.9	200	3.2	0.00	0.00	0.00	0.00	5
16 DEC	117	End Leaf	7214	3.17	16.9	251	3.5	0.11	0.00	0.00	0.00	5
19 JAN	151	Phys. Mat	9986	2.57	16.9	389	3.9	0.00	0.02	0.00	0.00	7
31 JAN	163	Harv. Mat	8655	0.17	16.9	358	4.1	0.00	0.17	0.00	0.00	8
31 JAN	163	Harvest	8655	0.17	16.9	358	4.1	0.00	0.00	0.00	0.00	8

OVERVIEW - Bloco de notas														
Arquivo Editar Formatar Exibir Ajuda														
Development Phase	Time Span days	Average Environment				Cumulative			Stress (0=Min, 1=Max Stress)					
		Temp Max °C	Temp Min °C	Solar Rad MJ/m2	Photop [day]	CO2 ppm	Rain mm	Evapo Trans mm	Water Photo synth	Nitrogen Photo synth	Phosphorus Photo synth	Growth		
Emergence -First Flower	49	23.3	13.5	13.4	12.01	380.0	375.2	134.3	0.000	0.001	0.000	0.019	0.000	0.000
First Flower-First Seed	22	26.6	16.0	19.3	13.05	380.0	97.0	97.2	0.000	0.000	0.000	0.000	0.000	0.000
First Seed - Phys. Mat.	74	30.1	18.5	22.8	13.76	380.0	540.6	382.3	0.026	0.056	0.000	0.007	0.000	0.000
Emergence - Phys. Mat.	145	27.3	16.5	19.1	13.06	380.0	1013	614	0.013	0.029	0.000	0.010	0.000	0.000
Planting to Harvest	163	27.4	16.4	19.3	13.02	380.0	1046	665	0.012	0.026	0.000	0.021	0.000	0.000

\*Resource Productivity  
Growing season length: 163 days

Precipitation during growing season	1045.6 mm[rain]	
Dry Matter Productivity	0.83 kg[DM]/m3[rain]	= 8.3 kg[DM]/ha per mm[rain]
Yield Productivity	0.51 kg[grain yield]/m3[rain]	= 5.1 kg[yield]/ha per mm[rain]
Evapotranspiration during growing season	665.5 mm[ET]	
Dry Matter Productivity	1.30 kg[DM]/m3[ET]	= 13.0 kg[DM]/ha per mm[ET]
Yield Productivity	0.80 kg[grain yield]/m3[ET]	= 8.0 kg[yield]/ha per mm[ET]
Transpiration during growing season	443.3 mm[EP]	
Dry Matter Productivity	1.95 kg[DM]/m3[EP]	= 19.5 kg[DM]/ha per mm[EP]
Yield Productivity	1.20 kg[grain yield]/m3[EP]	= 12.0 kg[yield]/ha per mm[EP]
N uptake during growing season	78 kg[N uptake]/ha	
Dry Matter Productivity	111.0 kg[DM]/kg[N uptake]	
Yield Productivity	68.1 kg[yield]/kg[N uptake]	

Soybean YIELD : 5313 kg/ha [Dry weight]



PlantGro - Bloco de notas																
Arquivo Editar Formatar Exibir Ajuda																
@YEAR	DOY	DAS	DAP	L#SD	GSTD	L AID	LWAD	SWAD	GWAD	RWAD	VWAD	CWAD	G#AD	GWGD	HIAD	PWAD
2012	234	35	0	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	235	36	1	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	236	37	2	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	237	38	3	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	238	39	4	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	239	40	5	0.0	0	0.000	0	0	0	0	0	0	0	0.0	0.000	0
2012	240	41	6	0.0	0	0.023	12	3	0	14	14	14	0	0.0	0.000	0
2012	241	42	7	0.1	0	0.025	13	3	0	15	15	15	0	0.0	0.000	0
2012	242	43	8	0.1	0	0.028	14	3	0	15	17	17	0	0.0	0.000	0
2012	243	44	9	0.2	0	0.032	15	3	0	15	18	18	0	0.0	0.000	0
2012	244	45	10	0.3	0	0.037	17	3	0	16	20	20	0	0.0	0.000	0
2012	245	46	11	0.4	0	0.043	19	4	0	17	22	22	0	0.0	0.000	0
2012	246	47	12	0.5	0	0.050	21	4	0	19	25	25	0	0.0	0.000	0
2012	247	48	13	0.6	0	0.055	22	4	0	21	27	27	0	0.0	0.000	0
2012	248	49	14	0.7	0	0.060	25	5	0	23	29	29	0	0.0	0.000	0
2012	249	50	15	0.8	0	0.068	26	6	0	26	32	32	0	0.0	0.000	0
2012	250	51	16	0.9	0	0.074	27	6	0	28	34	34	0	0.0	0.000	0
2012	251	52	17	1.1	0	0.095	32	7	0	30	39	39	0	0.0	0.000	0
2012	252	53	18	1.3	0	0.115	37	7	0	31	44	44	0	0.0	0.000	0
2012	253	54	19	1.5	0	0.131	40	8	0	32	48	48	0	0.0	0.000	0
2012	254	55	20	1.6	0	0.143	43	8	0	33	51	51	0	0.0	0.000	0
2012	255	56	21	1.7	0	0.160	48	9	0	35	56	56	0	0.0	0.000	0
2012	256	57	22	1.9	0	0.179	52	10	0	39	62	62	0	0.0	0.000	0
2012	257	58	23	2.1	0	0.192	58	11	0	41	69	69	0	0.0	0.000	0
2012	258	59	24	2.3	0	0.223	69	12	0	44	81	81	0	0.0	0.000	0
2012	259	60	25	2.5	0	0.256	72	12	0	45	85	85	0	0.0	0.000	0
2012	260	61	26	2.7	0	0.297	77	13	0	47	90	90	0	0.0	0.000	0
2012	261	62	27	3.0	0	0.337	82	15	0	51	98	98	0	0.0	0.000	0
2012	262	63	28	3.2	0	0.372	87	16	0	51	103	103	0	0.0	0.000	0
2012	263	64	29	3.3	0	0.392	97	17	0	56	114	114	0	0.0	0.000	0
2012	264	65	30	3.4	0	0.405	105	19	0	58	124	124	0	0.0	0.000	0
2012	265	66	31	3.5	0	0.423	116	20	0	61	136	136	0	0.0	0.000	0
2012	266	67	32	3.6	0	0.439	125	22	0	63	147	147	0	0.0	0.000	0
2012	267	68	33	3.7	0	0.458	135	23	0	65	159	159	0	0.0	0.000	0
2012	268	69	34	3.9	0	0.508	154	30	0	73	184	184	0	0.0	0.000	0