

NOVA METODOLOGIA DE ANÁLISE DE SOLO COM BASE EM INFRAVERMELHO PARA DETERMINAÇÕES DE ROTINA EM LARGA ESCALA

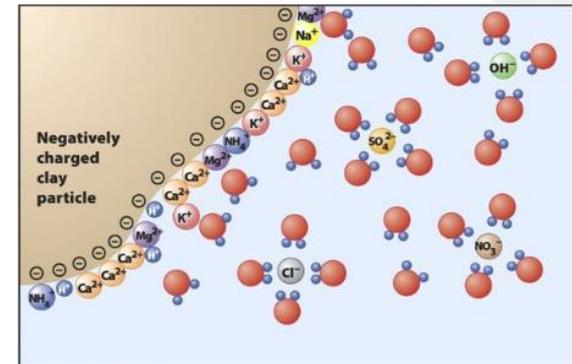
Daniel Vidal Pérez & André Marcelo de Souza



Componentes Ativos do Solo

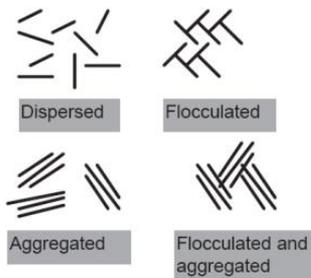
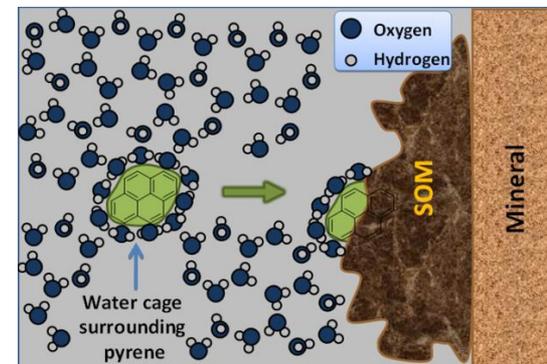
Possuem carga elétrica de SUPERFÍCIE

- » Adsorção de água;
- » Adsorção de nutrientes
- » Adsorção de POLUENTES
- » Expansão e Contração
- » Pegajosidade e Plasticidade, etc.....



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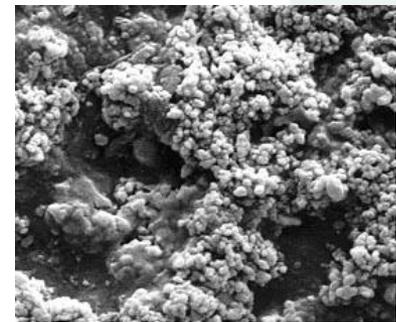
Componentes Ativos do Solo

Basicamente 2 componentes

» *Coloides Orgânicos ou Substâncias Húmicas*

Provêm da humificação da matéria orgânica:

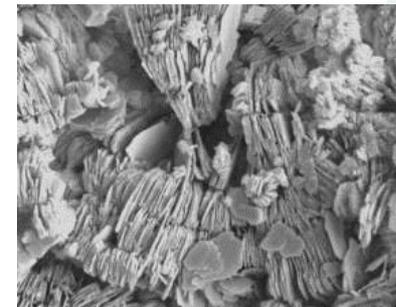
Ácidos Fúlvicos, Ácidos Húmicos, Humina



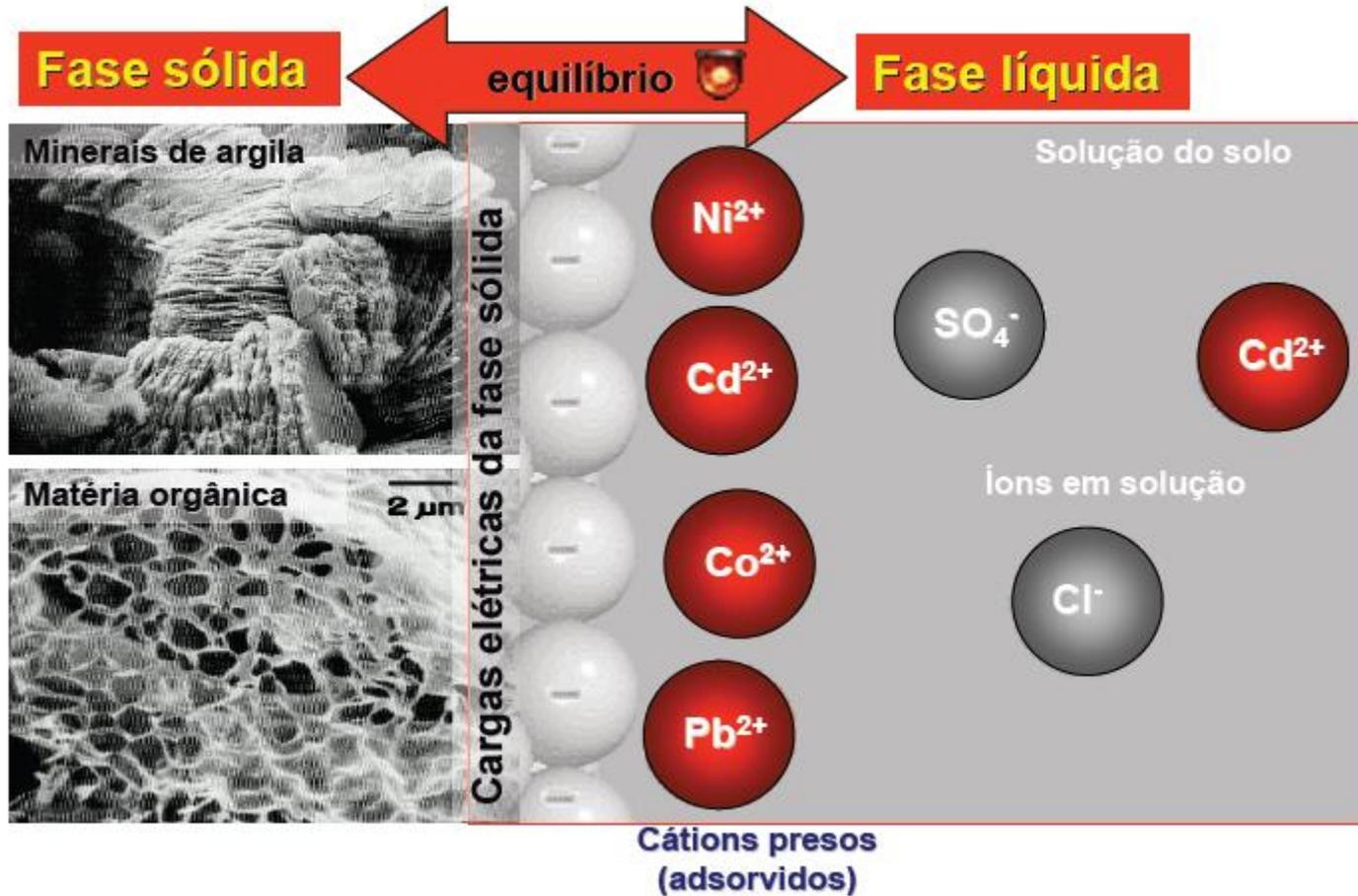
SEM image (approx 2000 times enlarged) of a solid humic acid (www.hagroup.neu.edu)

» *Coloides Minerais ou Argila*

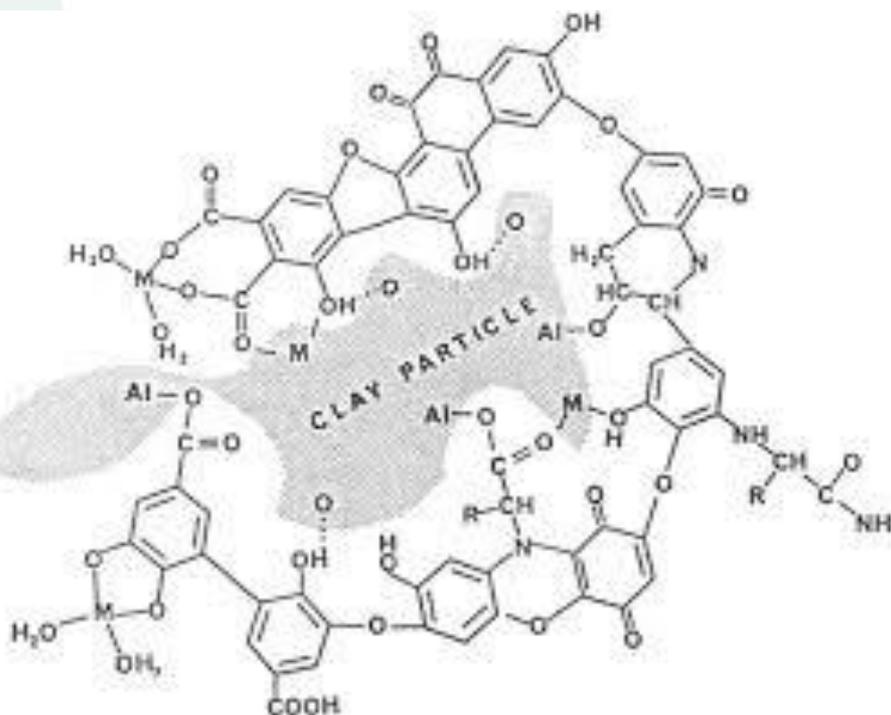
Provêm do Intemperismo



Componentes Ativos do Solo



Componentes Ativos do Solo

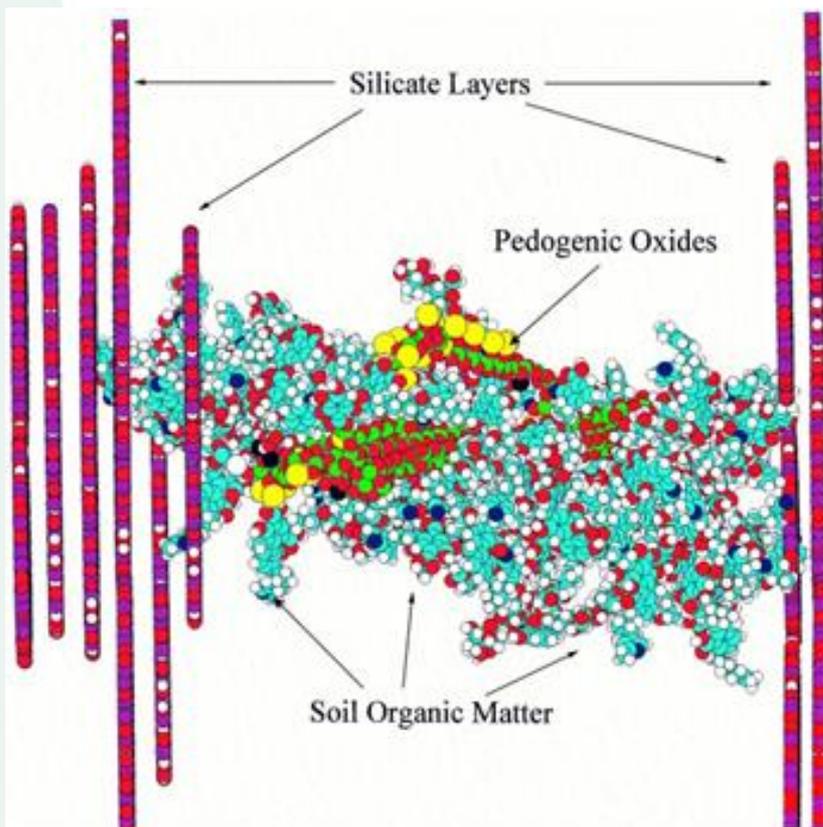


Componente	Área Superficial ^a	CTC pH 7,0 ^b
	m ² g ⁻¹	cmol _c kg ⁻¹
Caulinita	7-30	8
Óxidos Fe/Al	5-70	4
Substâncias Húmicas	700-800	200
Vermiculita	400-800	150
Esmectita	600-800	100
Ilita	60-200	30

a. Alleoni et al. 2009. pag. 72 [Melo & Alleoni, 2009, Parte 2]

b. Lepsch. 2011. pag.115.

Componentes Ativos do Solo



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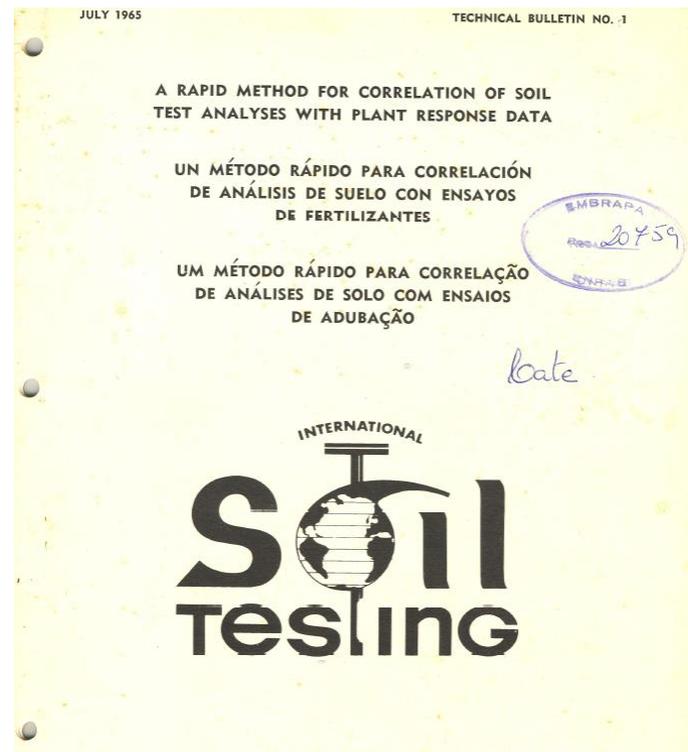
a. Alleoni et al. 2009. pag. 72 [Melo & Alleoni, 2009, Parte 2]

b. Lepsch. 2011. pag.115.

Análise de Solo no Brasil - 1965

INTERNATIONAL SOIL FERTILITY EVALUATION & IMPROVEMENT PROGRAM

Desenvolver competências na avaliação de problemas de fertilidade de solo através da análise de solo e experimentação



Análise de Solo no Brasil - 1969

ANÁLISES PARA FINS DE FERTILIDADE MÉTODOS ANALÍTICOS A SEREM EXECUTADOS DENTRO DO PRORAMA NACIONAL DE FERTILIDADE DO SOLO

Boletim Técnico n.º 7

EQUIPE DE PEDOLOGIA E FERTILIDADE DO SOLO

EPE — MINISTÉRIO DA AGRICULTURA

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MÉTODOS DE ANÁLISE DE SOLO

LEANDRO VETTORI *

Pesquisador em Química

* Bolsista do CNPq.

Análise de Solo no Brasil



MÉTODO DE REFERÊNCIA

Processo longo e trabalhoso

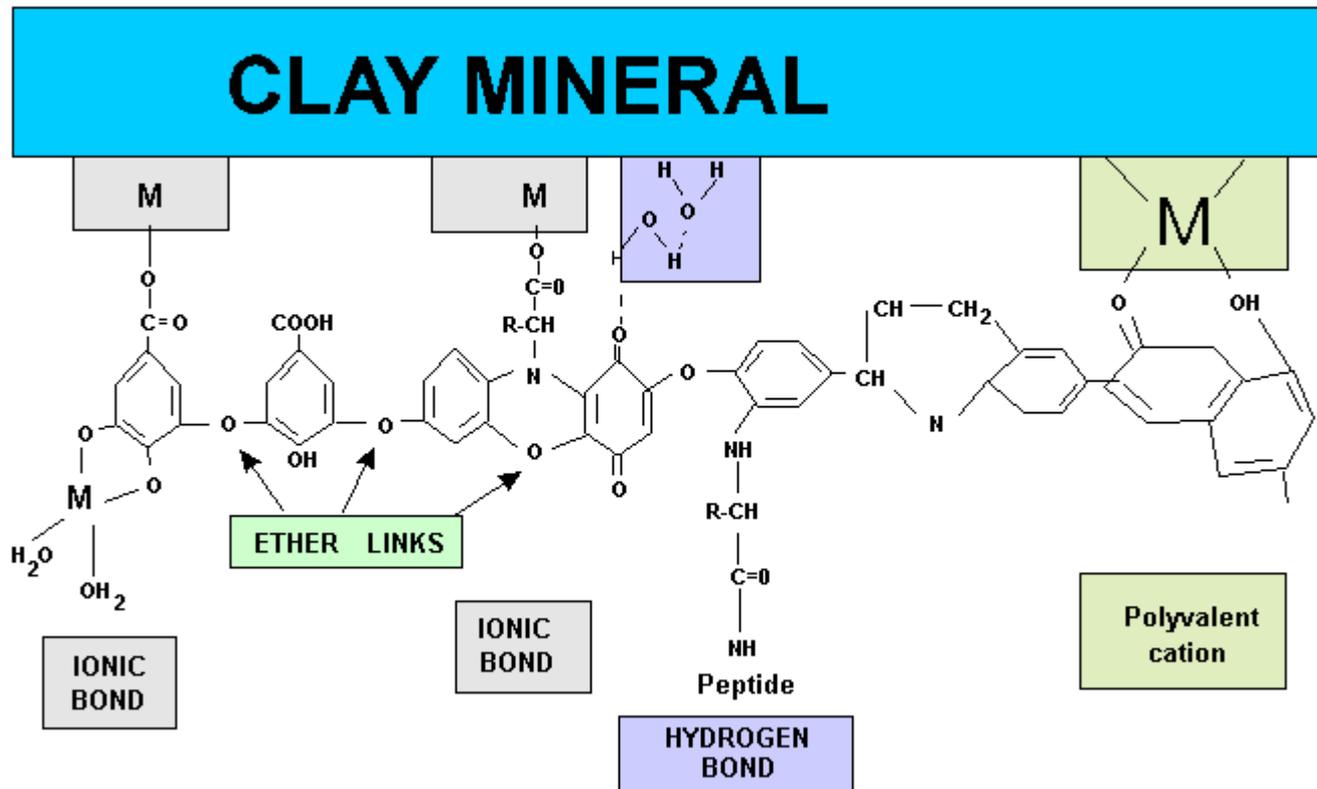
Geradora de resíduos

LABORATÓRIO DE SOLO

Demanda mão-de-obra qualificada e numerosa

Possibilidade de impacto ambiental.

Componentes Ativos do Solo

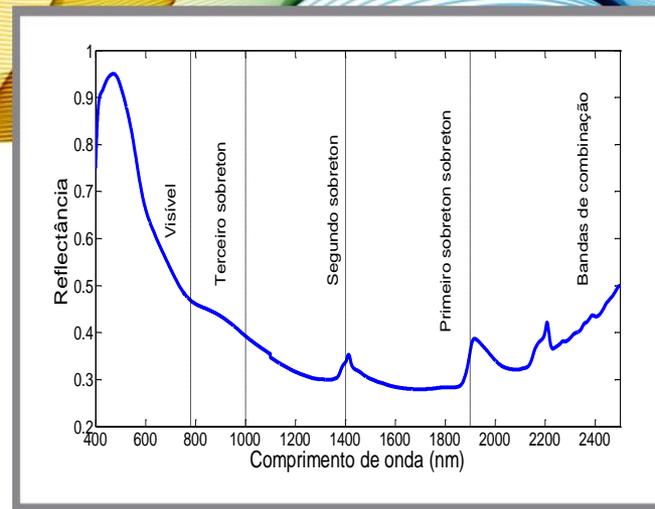


Espectroscopia Infravermelho

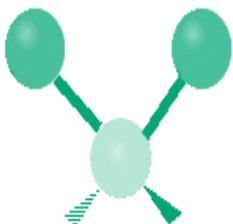
As ligações entre os átomos que formam as moléculas possuem frequências específicas de vibração, que variam de acordo com a estrutura, composição e o modo de vibração da amostra.

- » Um espectrograma no infravermelho possui uma apresentação bidimensional das características de uma molécula;
- » Estas características aparecem como bandas ou picos, e podem ser descritas através de três variáveis: posição, intensidade e formato. Os dois primeiros podem ser expressos em números;
- » Foi usada primeiramente para materiais orgânicos, mas também se aplica a inorgânicos.

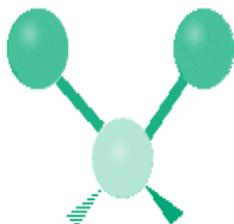
- ✓ **12500 – 4000 cm^{-1} ou 800 - 2500nm;**
- ✓ **Sobretons + banda de combinação;**
- ✓ **C-H, N-H, O-H, S-H;**
- ✓ **Poucos intensas e sobrepostas**



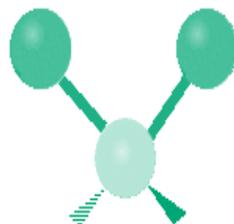
Princípio da Técnica . Modos Vibracionais



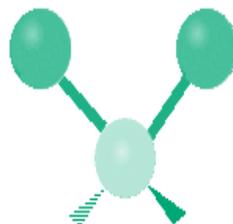
Symmetric
Stretching



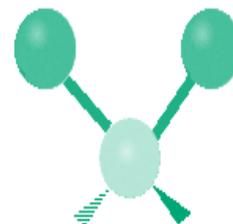
Antisymmetric
Stretching



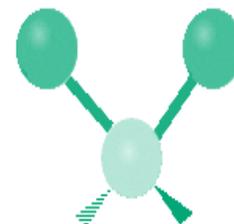
Scissoring



Rocking

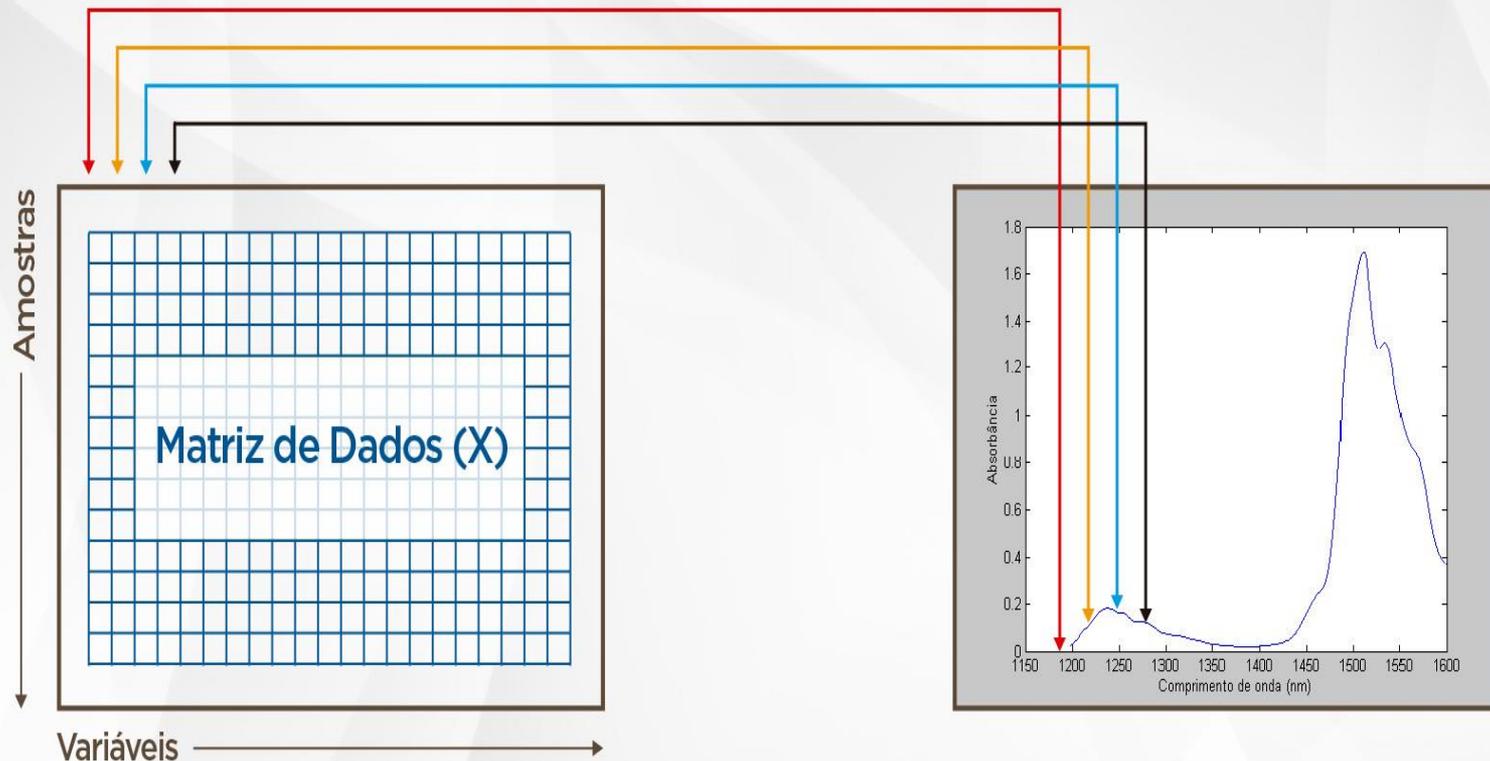


Wagging

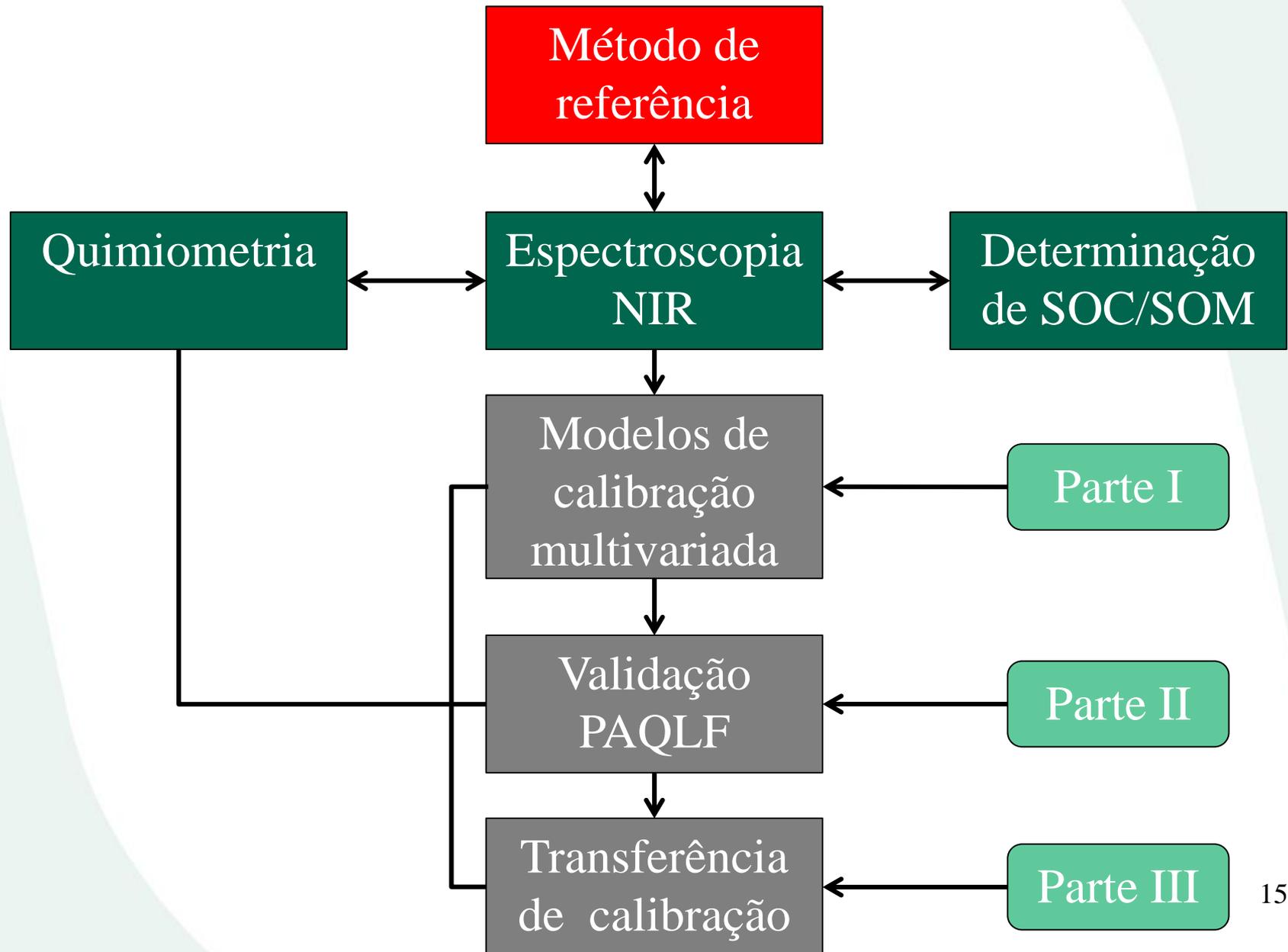


Twisting

▶ **Dados químicos multivariados (espectros) podem ser arranjados na forma de uma MATRIZ DE DADOS.**



Modelagem Experimental



Publicações Científicas

A.M. de Souza et al., *J. Near Infrared Spectrosc.* **24**, 293–303 (2016)

Received: 15 May 2015 ■ Revised: 4 March 2016 ■ Accepted: 12 May 2016 ■ Publication: 7 June 2016

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Special Issue: Near Infrared Spectroscopy of Soil

Validation of the near infrared spectroscopy method for determining soil organic carbon by employing a proficiency assay for fertility laboratories

André Marcelo de Souza,^{a*} Paulo Roberto Filgueiras,^b Maurício Rizzato Coelho,^a Ademir Fontana,^a Thayane Christine Barbosa Winkler,^a Patrícia Valderrama^c and Ronei Jesus Poppi^b

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Publicações Científicas

Article

<http://dx.doi.org/10.5935/0103-5053.20160031>

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0103 - 5053 \$6.00+0.00



Soil Organic Carbon Determination Using NIRS: Evaluation of Dichromate Oxidation and Dry Combustion Analysis as Reference Methods in Multivariate Calibration

Karla K. Beltrame,^a André M. Souza,^{,b} Maurício R. Coelho,^b Thayane C. B. Winkler,^b Wyrllen E. Souza^a and Patrícia Valderrama^{*,a}*

^a*Universidade Tecnológica Federal do Paraná, UTFPR, CP 271,
87301-899 Campo Mourão-PR, Brazil*

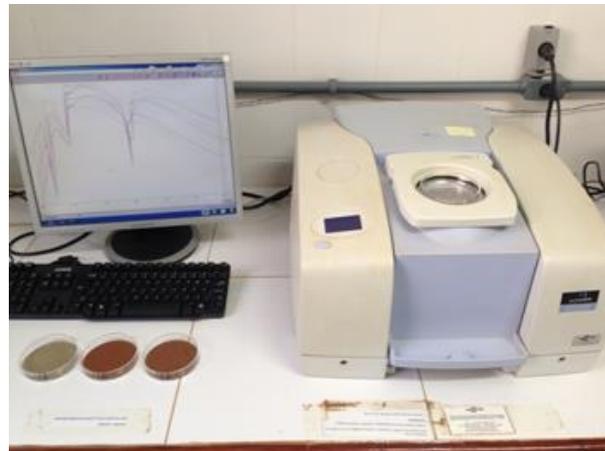
^b*Empresa Brasileira de Pesquisa Agropecuária, EMBRAPA Solos,
22460-000 Rio de Janeiro-RJ, Brazil*

Dichromate oxidation and dry combustion analysis were evaluated as reference methods to determine organic carbon in Brazilian soils using near infrared spectroscopy (NIRS) as an alternative. The main objective of this study was to evaluate which of the reference methods could provide a calibration model with higher predictive ability. A total of 161 soil samples obtained from horizons in full profiles (Parque Estadual da Mata Seca, Minas Gerais State, Brazil) were used. Models were mean centered and built from partial least squares. The dichromate oxidation method presented a lower accuracy when compared to dry combustion analysis as reference for NIRS. Figures of merit such as sensitivity, analytical sensitivity, detection and quantification limits, adjust and linearity presented results very similar. A paired *t*-test was applied to the figures of merit results and with 95% confidence did not show significant differences between the two methods

Espectroscopia Infravermelho

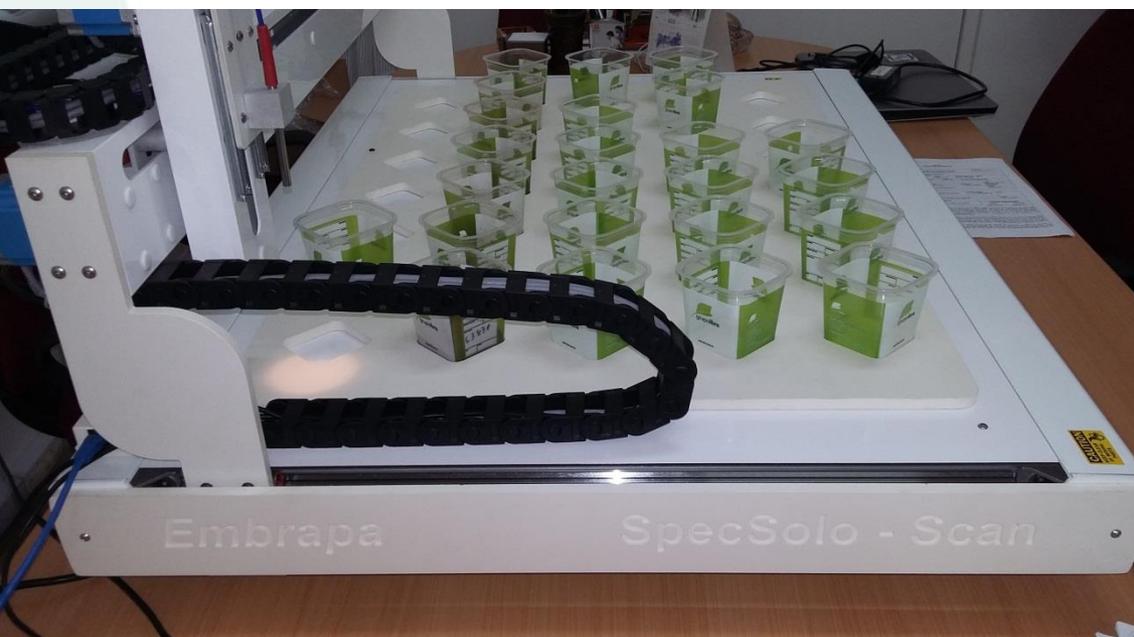
Problemas para entrar na Rotina

- » Custo equipamento \Rightarrow Importado;
- » Amostra \Rightarrow uma a uma;
- » Processamento dos espectros por especialista;
- » Cada um com seu banco de dados;
- » Equipamentos diferentes produzem resultados diferentes.



Espectroscopia Infravermelho

Solução para entrar na Rotina



SpecSolo Scan®



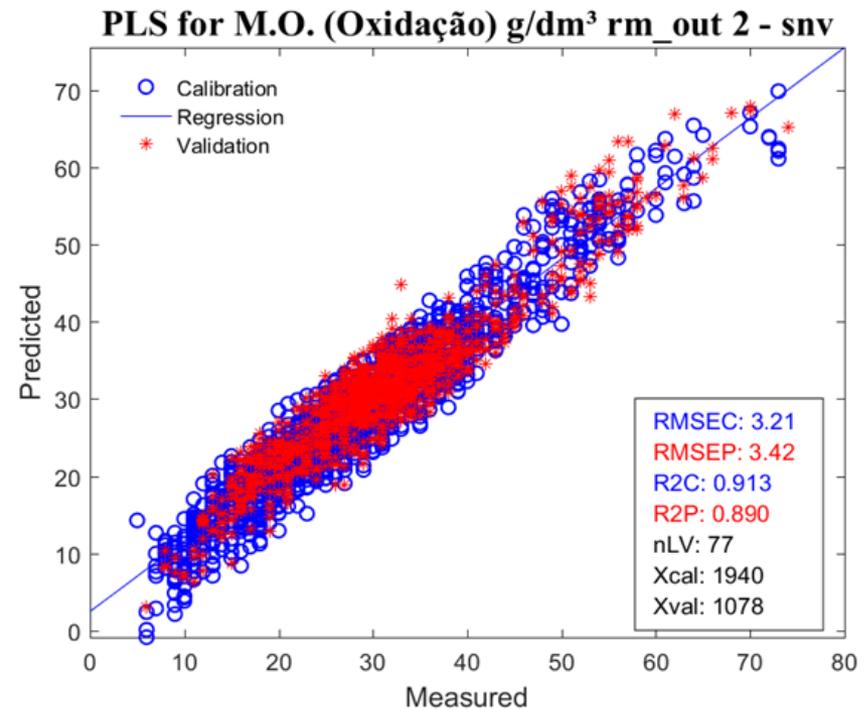
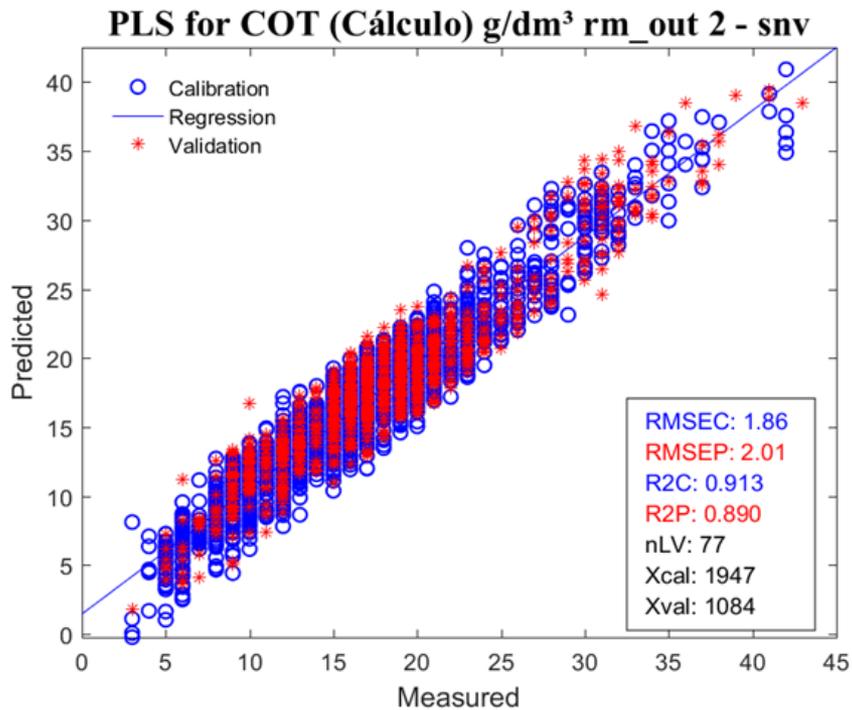
Espectroscopia Infravermelho

Solução para entrar na Rotina



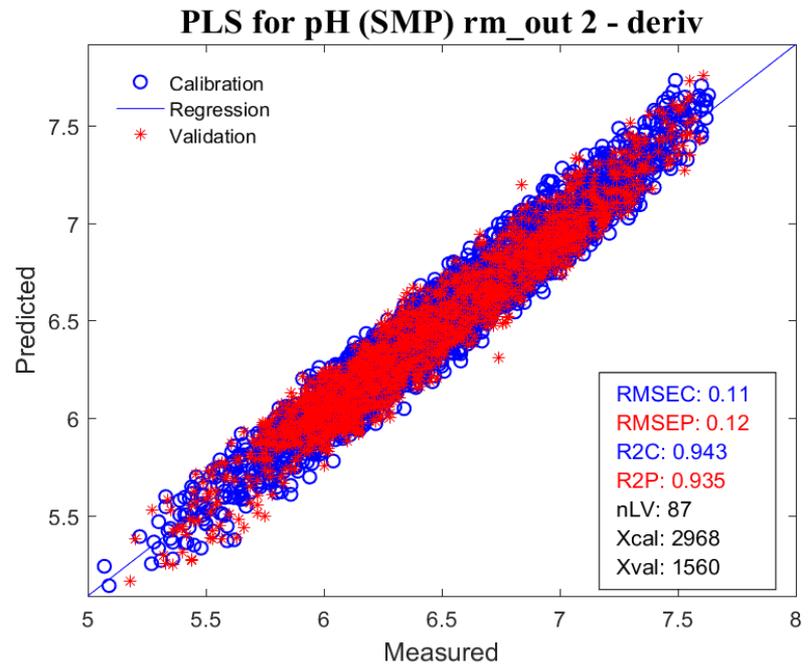
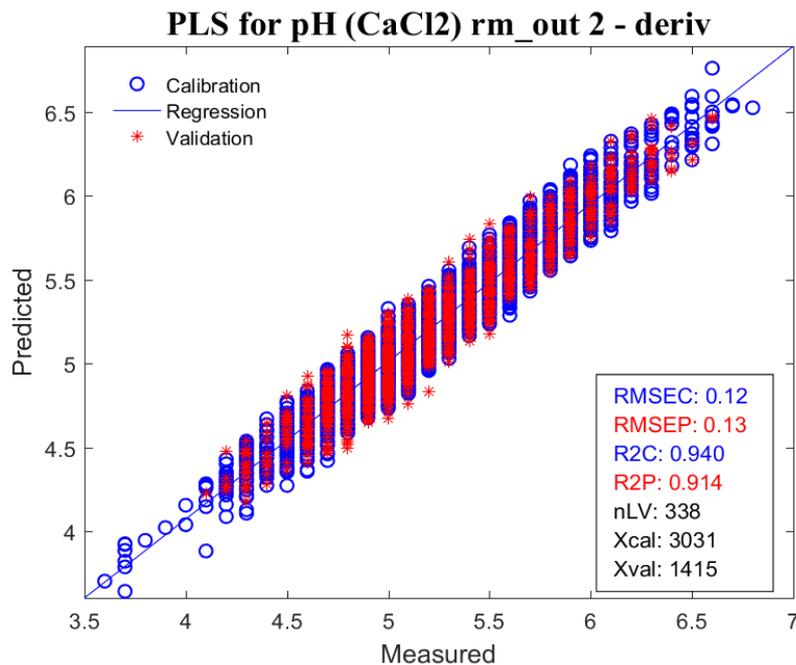
Principais Resultados

Modelo atual



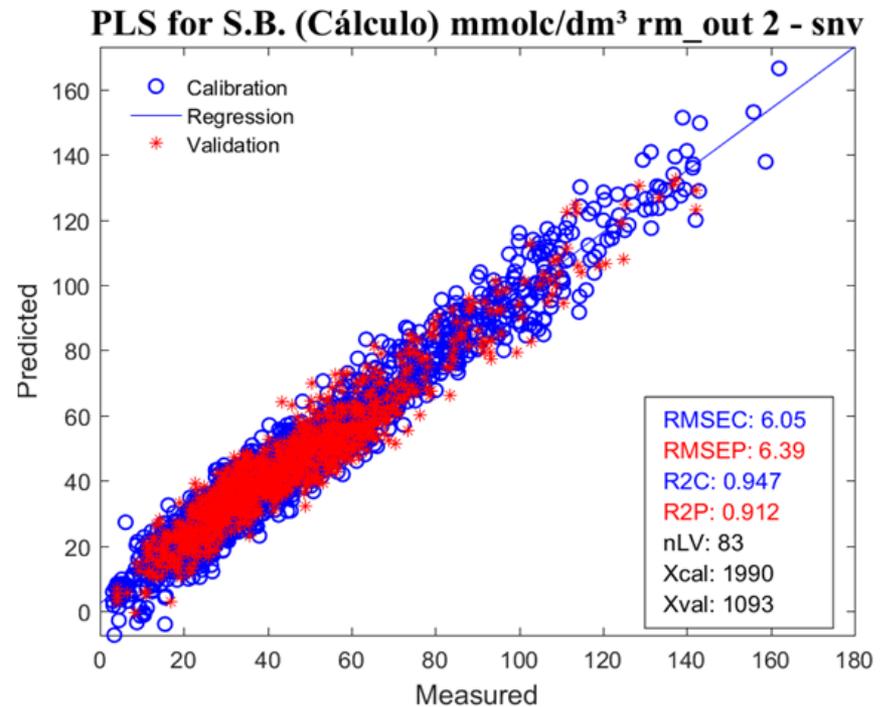
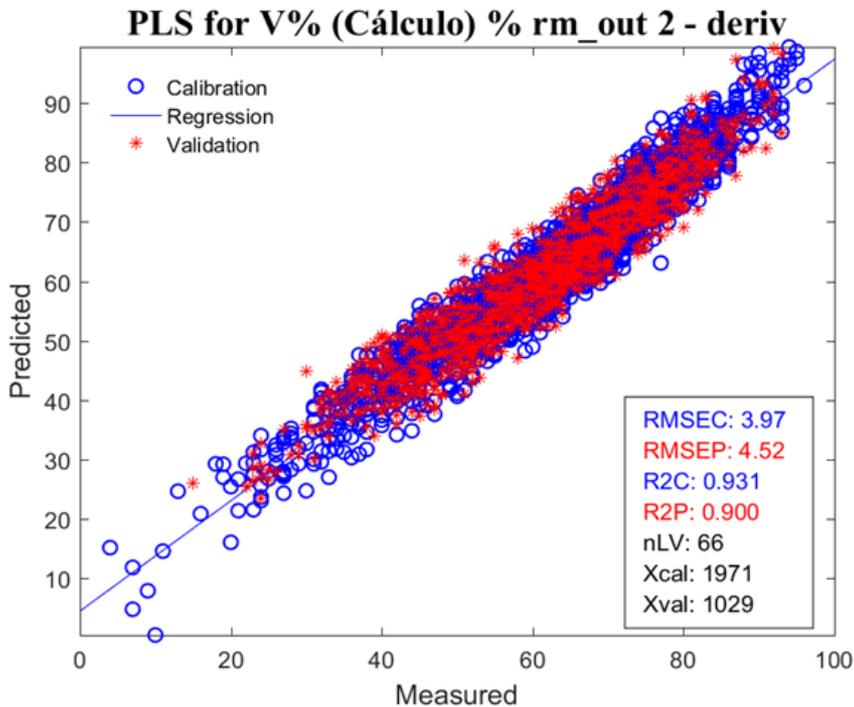
Principais Resultados

Modelo atual



Principais Resultados

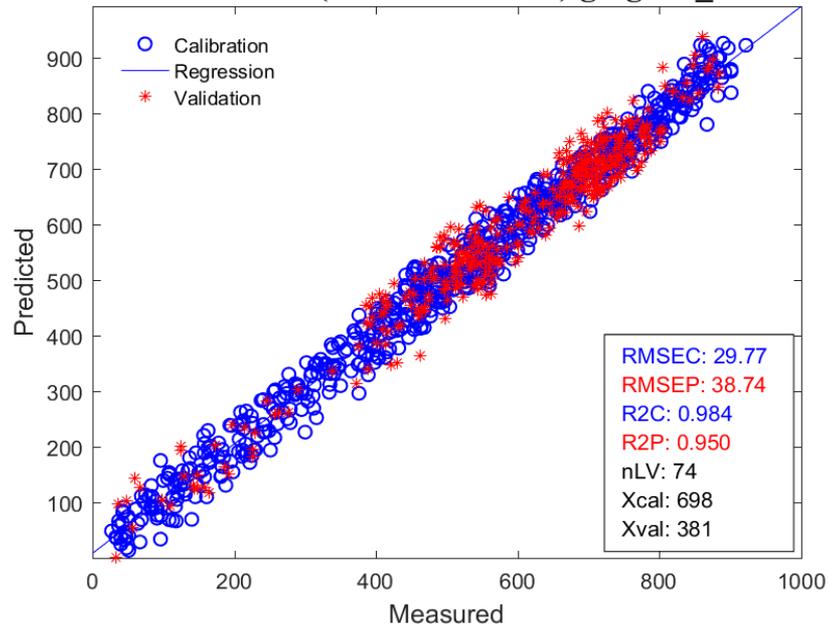
Modelo atual



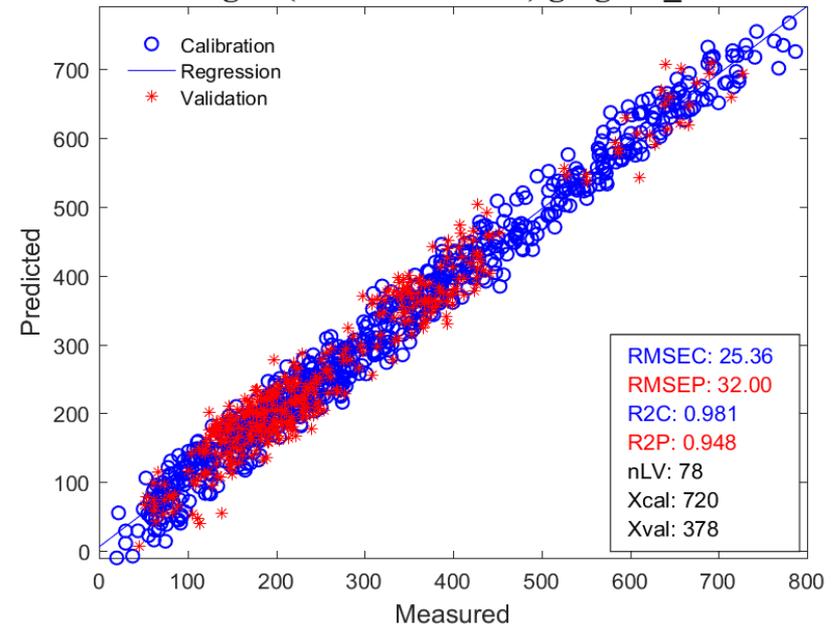
Principais Resultados

Modelo atual

PLS for Areia Total (HMFS + NaOH) g/kg rm_out 2 - auto

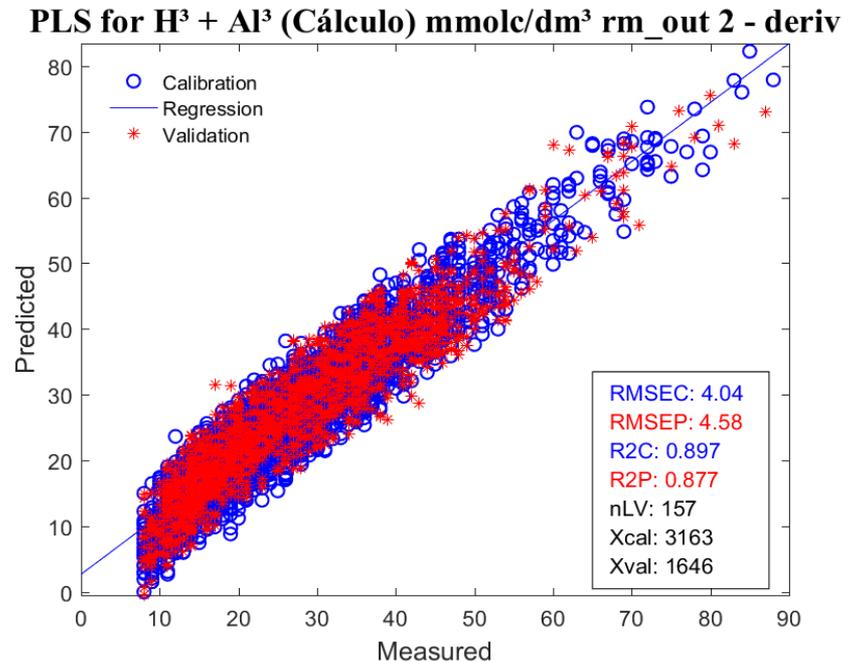
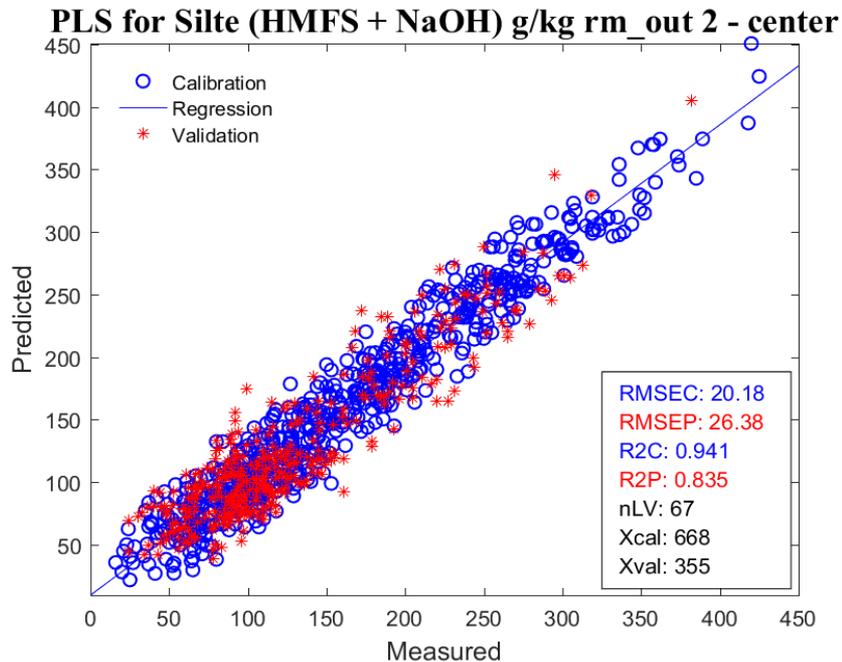


PLS for Argila (HMFS + NaOH) g/kg rm_out 2 - auto



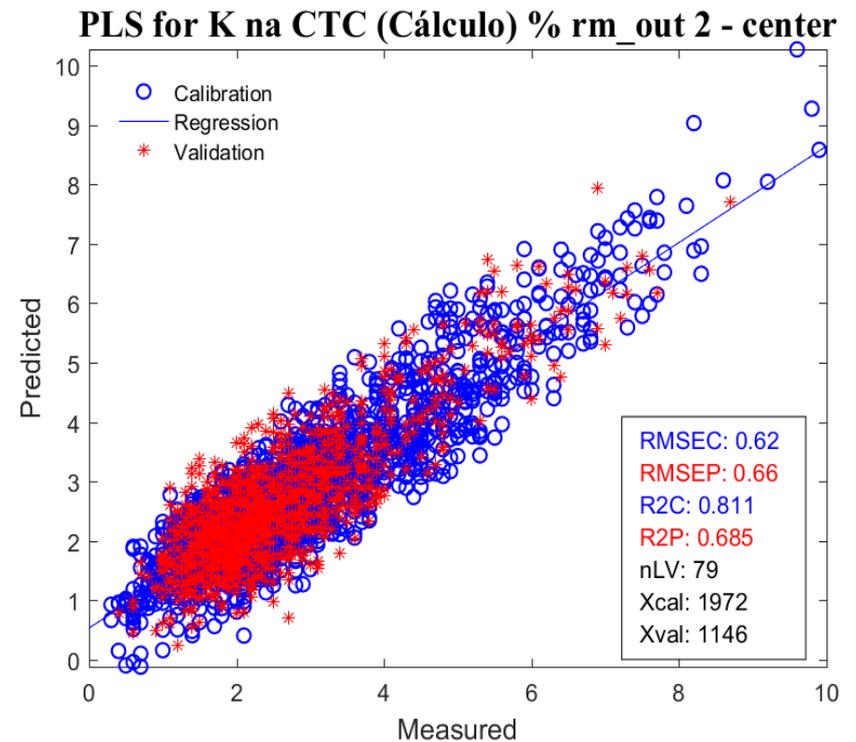
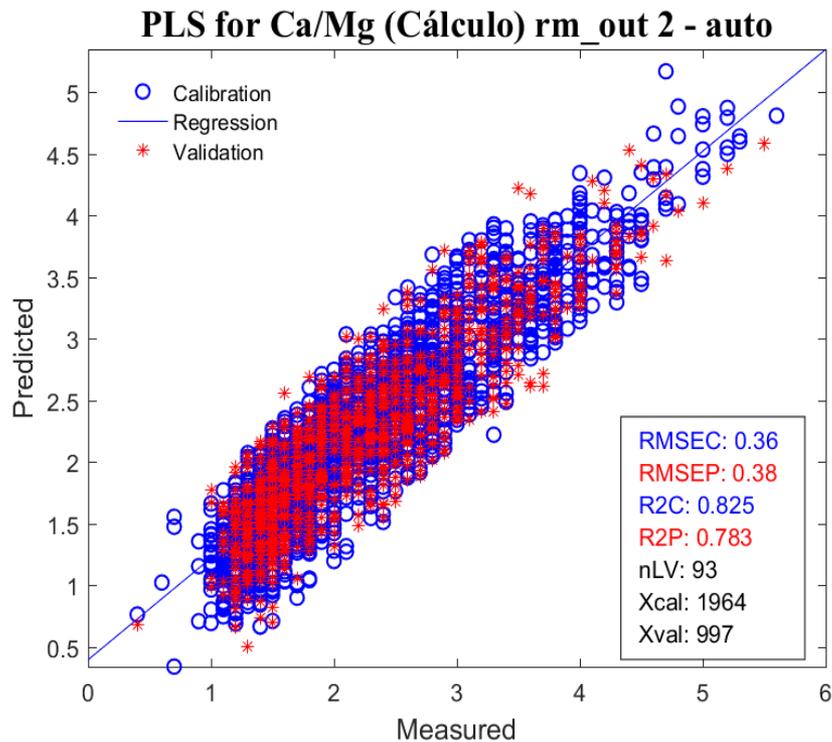
Principais Resultados

Modelo Atual



Principais Resultados

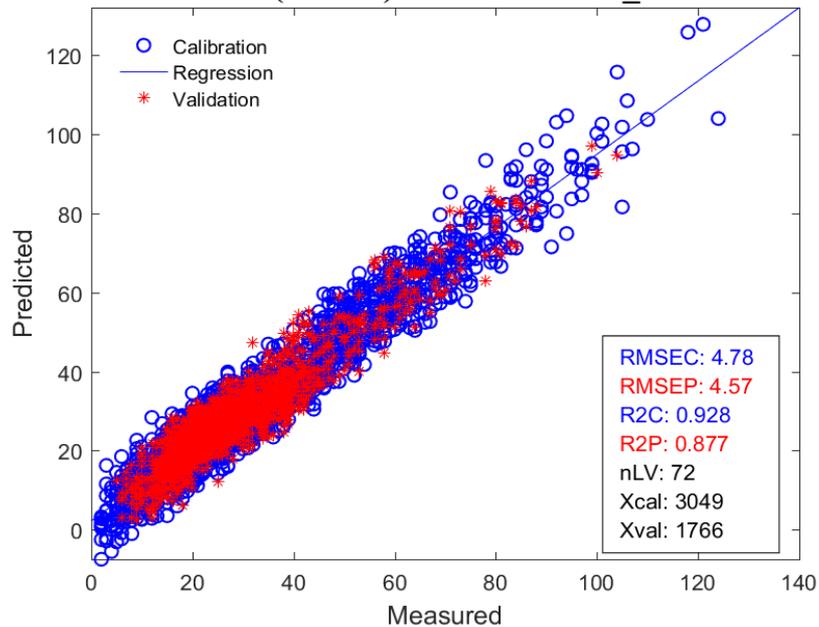
Modelo Atual



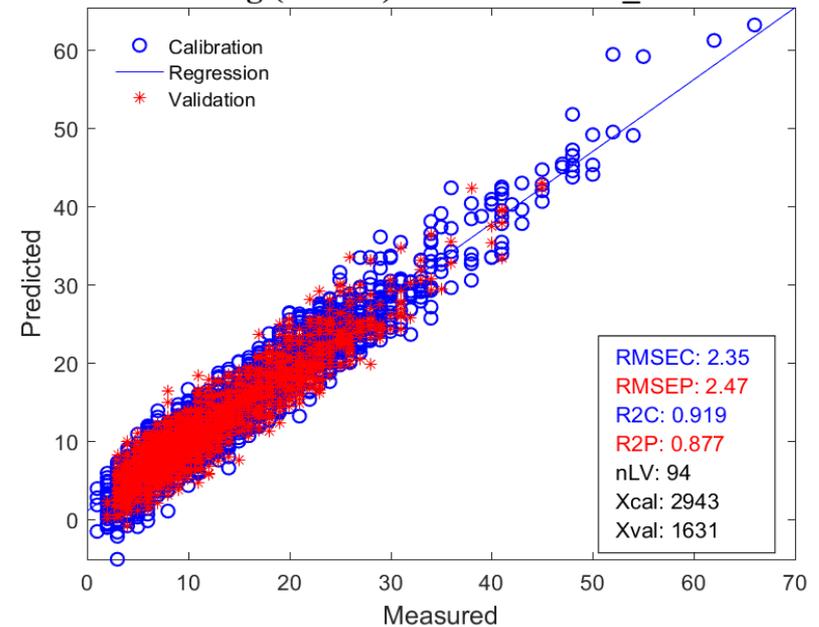
Principais Resultados

Modelo Atual

PLS for Ca (Resina) mmolc/dm³ rm_out 2 - snv

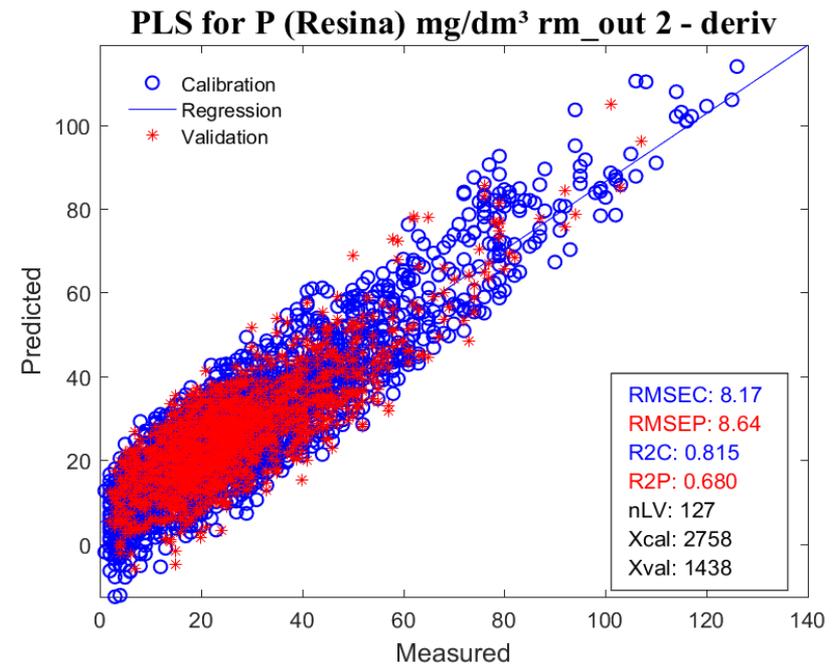
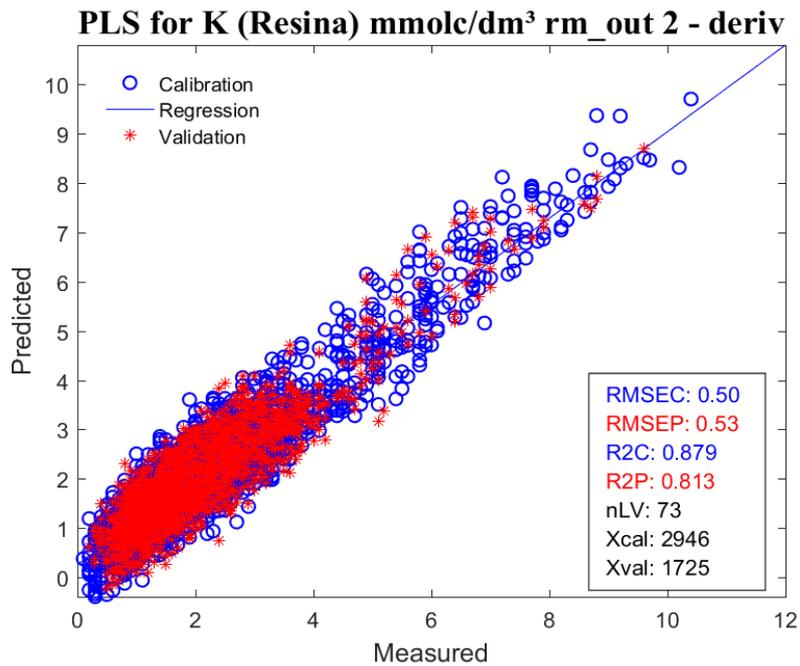


PLS for Mg (Resina) mmolc/dm³ rm_out 2 - snv



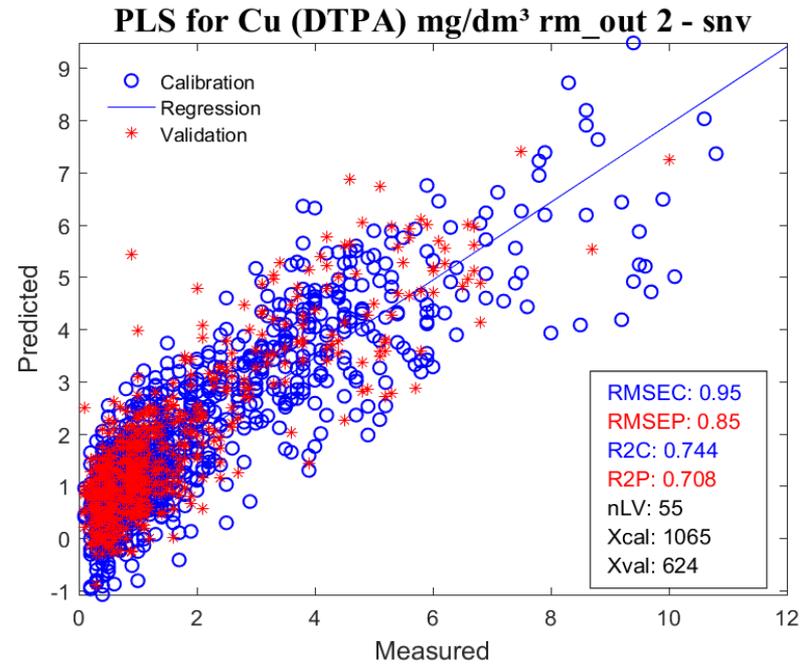
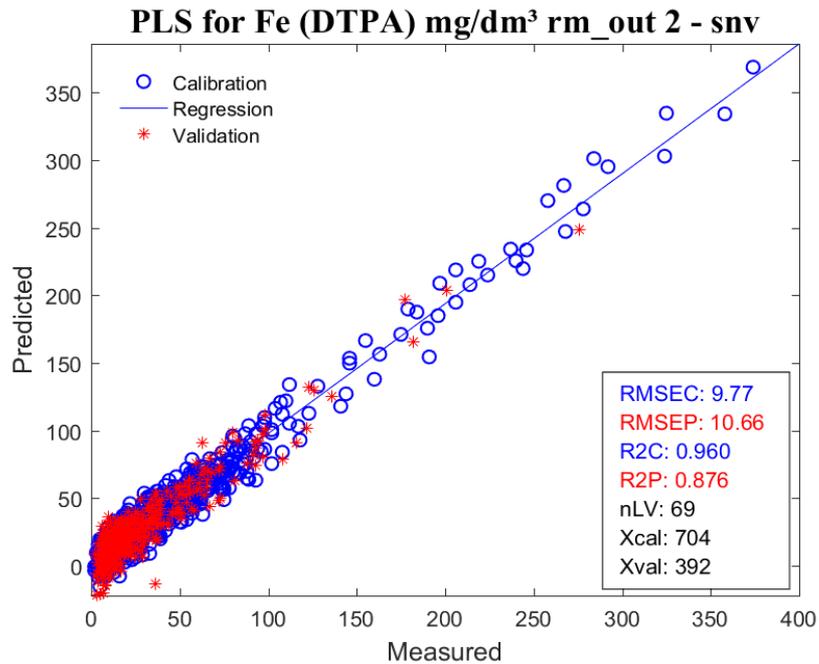
Principais Resultados

Modelo Atual



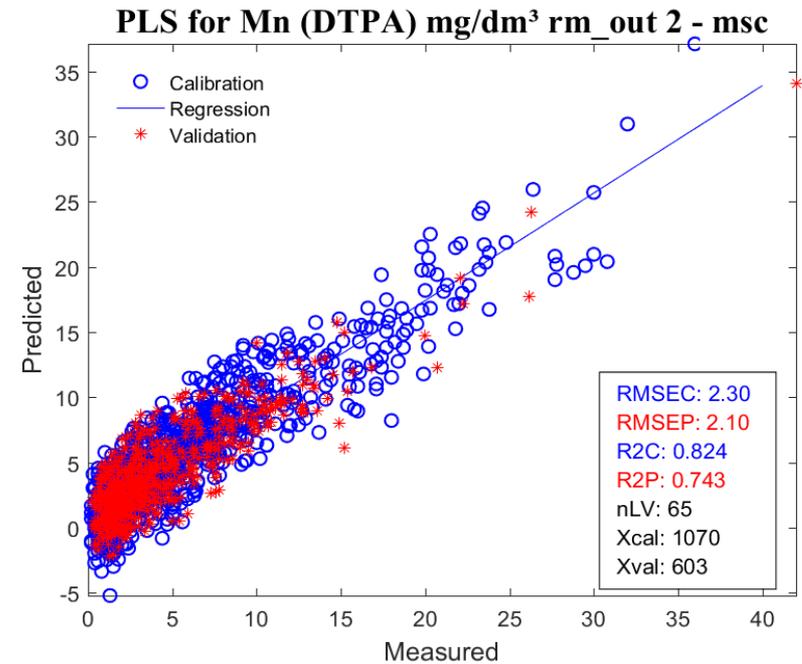
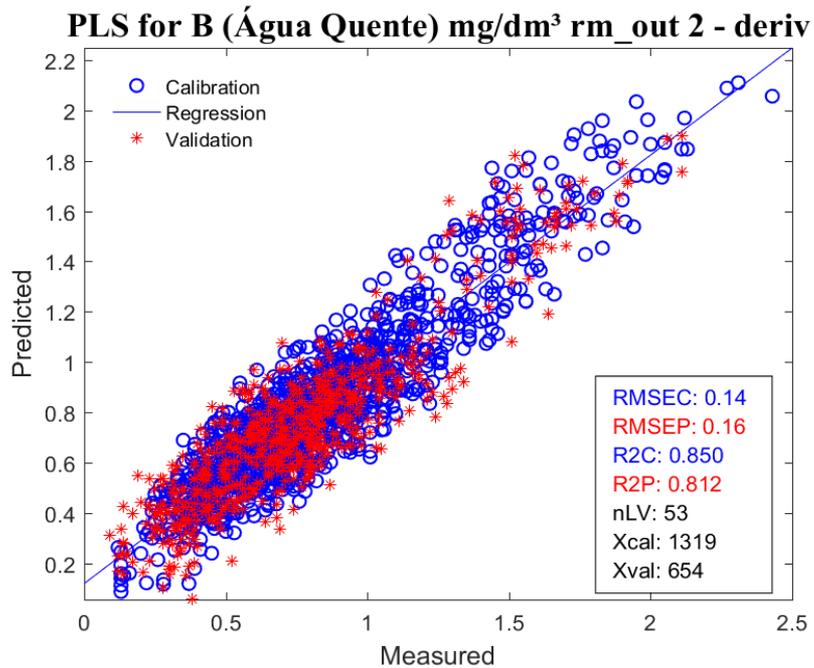
Principais Resultados

Modelo Atual



Principais Resultados

Modelo Atual



Perspectivas Futuras

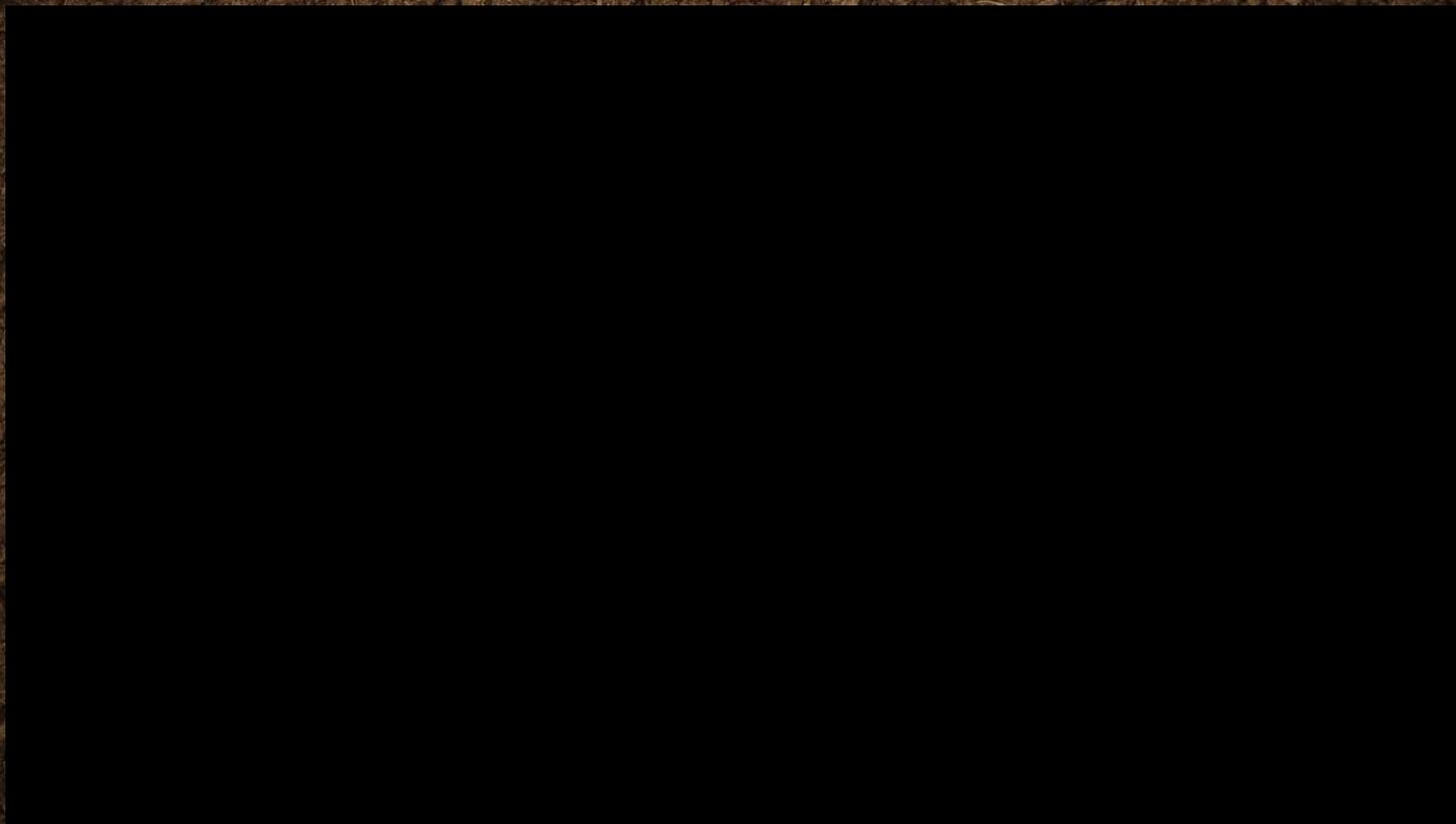


Base de dados:

Embrapa Solos / SpecLab conta com acesso à mais de **1 milhão de amostras** recuperadas de todas as regiões do Brasil.

Isto nos dá a possibilidade de desenvolver **calibrações com grande atribuição de variabilidade natural**.

Princípio de funcionamento da tecnologia





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Embrapa Solos

www.embrapa.br/solos



MINISTÉRIO DA
AGRICULTURA, PECUÁRIA
E ABASTECIMENTO



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