ATC-STA Seminar-Discussion

Mathematical Modelling in Seed Testing

Introduction to the initiative and types of modelling to consider

Presenter: Bert van Duijn / Tomoko Sakata
Location: Verona, Italy
Date: May 31, 2023

From ATC initiative to Inter-Committee working goup

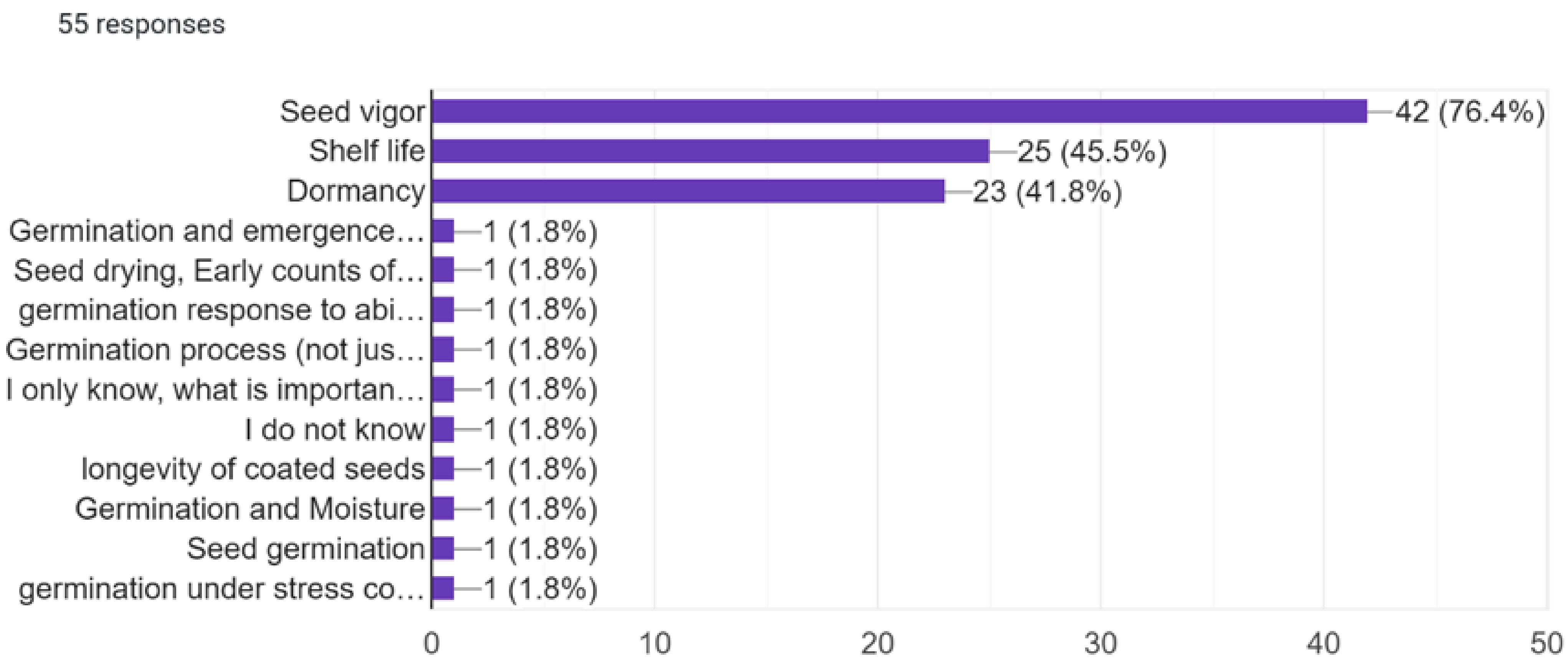
- Establishment (2021) of ATC working group “Mathematical Modeling” started to explore the role and possibilities of Mathematical Modeling in Seed Testing.

- Inventory of “all” scientific papers on Mathematical Modeling on Seeds.

- Inventory of needs and idea’s on the topic of ISTA committee members.

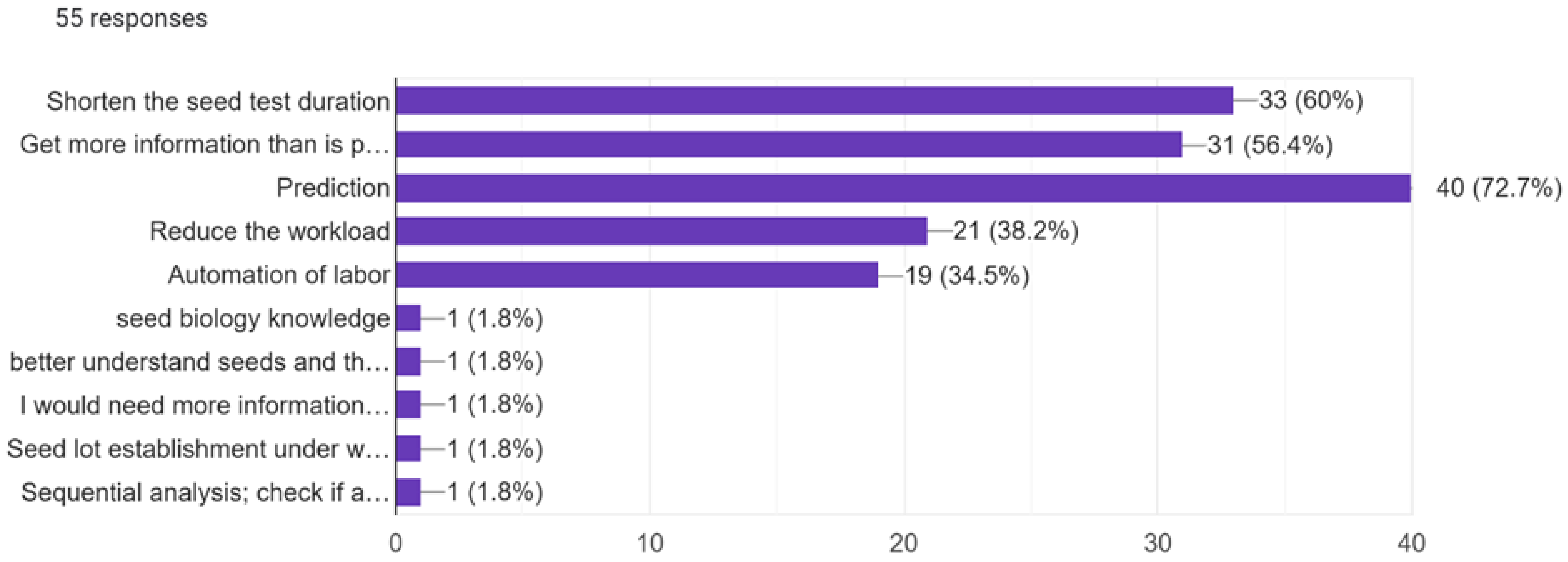
From ATC initiative to Inter-Committee working goup

Survey results: **What are the most interesting areas to apply (mathematical) modelling?**



From ATC initiative to Inter-Committee working goup

Survey results: **What do you foresee as the purpose of application of (mathematical) modelling?**



From ATC initiative to Inter-Committee working goup

- Survey indicated that the majority of the other committee members is interested in the "Mathematical modelling" in connection to seed testing.
- Based this we enlarged the working group with more specialists from other committees and make decisions on the focus for specific type(s) of modelling as well as seed testing application fields.

Current inter-committee working group:

Tomoko Sakata, Kent Bradford, Bert van Duijn (ATC)
Kirk Remund, Jean-Louis Laffont (STA)
Fiona Hay (MOI and SST)

From ATC initiative to Inter-Committee working goup

Aims

- Explore the role and possibilities of Mathematical Modeling in Seed Testing and inform Technical Committees and the ISTA community.
- To assist ISTA by formulating views on(future) Mathematical Modeling developments from a seed testing perspective.
- Organize “Interest Group” meetings at ISTA Meetings.
- Organizing ISTA Workshop(s) on Mathematical Modeling
- Explore possibilities for an ISTA special project

Mathematical models

What do we mean with “mathematical modelling” in relationship to Seed testing, e.g. what type of models/ modelling do we want to include?

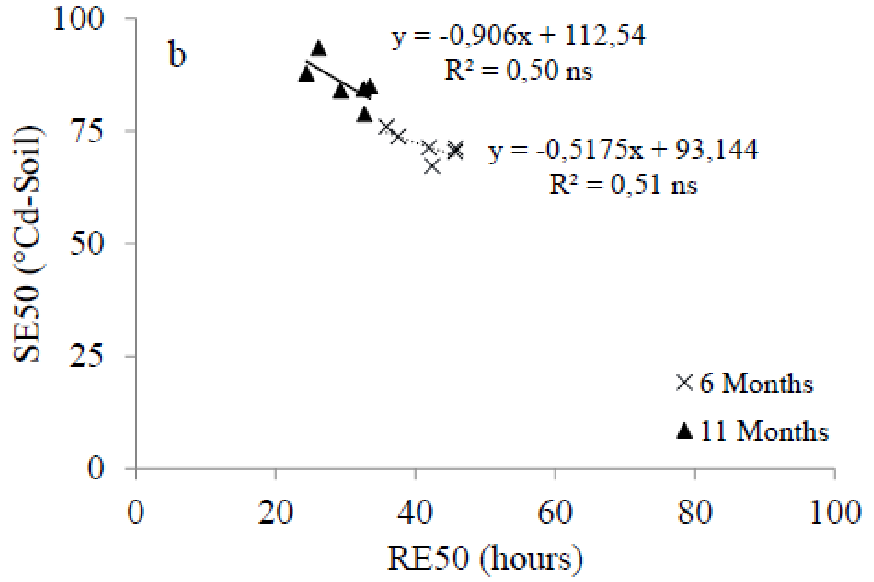
Types of Mathematical Models *(so far considered)*

- **Correlative models.**
- **(ODE) based models with “real” (is measurable physical and chemical) parameters.**
- **A.I. and neuronal network models (specially in image analysis)**
- **Statistical models and statistics in modelling.**

Short notes on Mathematical models

Correlative models

- Used mostly without the realisation that it is modelling (fitting a linear line through a collection of data points! why?)
- Used to detect correlations between measured parameter values and test it statistically
- Does not reveal causal relationships



From: Szemruch Cyntia et al. / IJAES, 8(1), 32-41, 2021

Mathematical model used:

Seedling emergence = a. radicle emergence +b

Short notes on Mathematical models

ODE (and PDE) models

- **Models describing the assumed (mechanistic) process based on physical and chemical parameters.**
- **Include the dynamics of the process (time and space dependent processes).**
- **Can reveal causal relationships and helps to understand "how it works"**

H. Liu et al./Journal of Theoretical Biology 427 (2017) 10–16

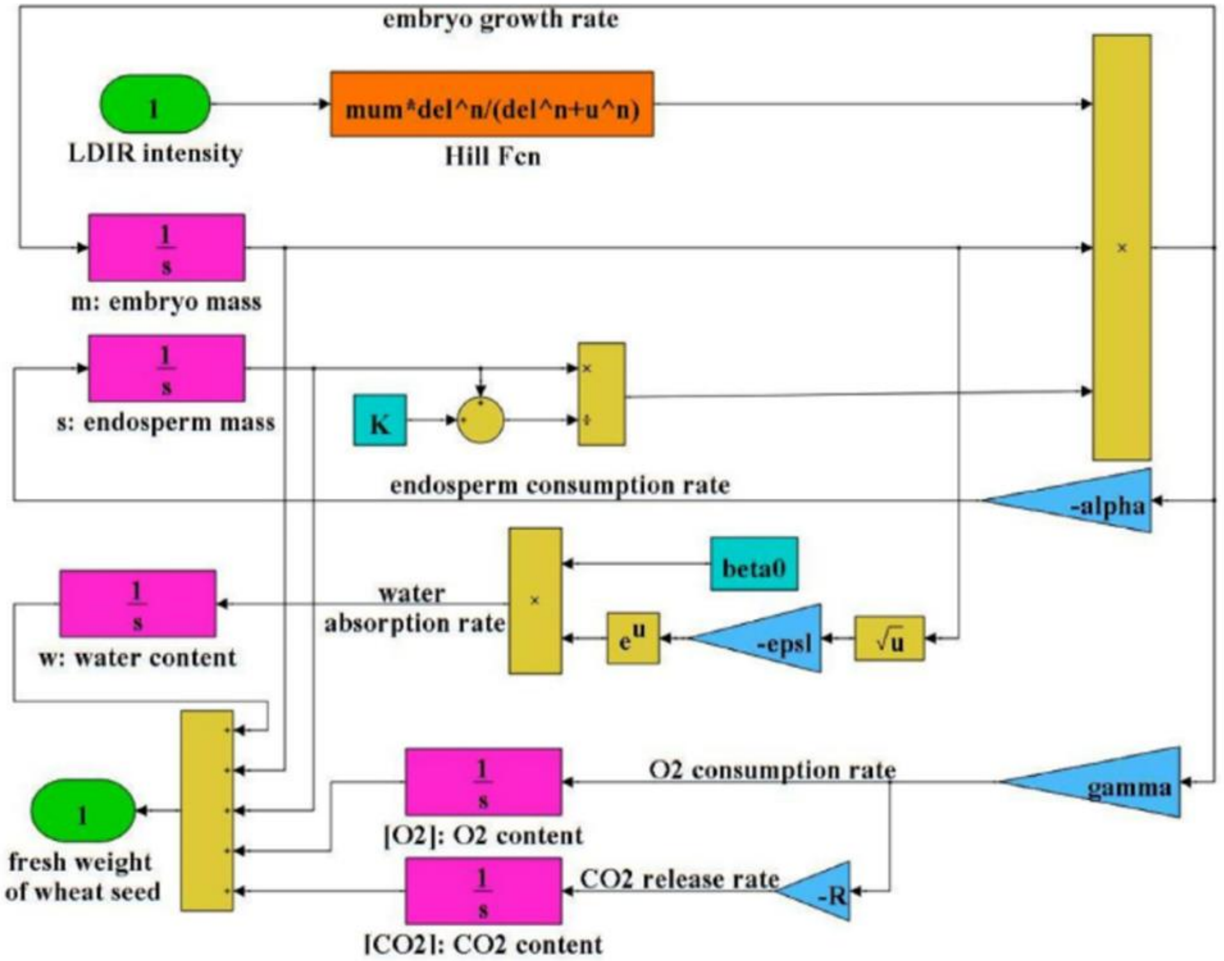
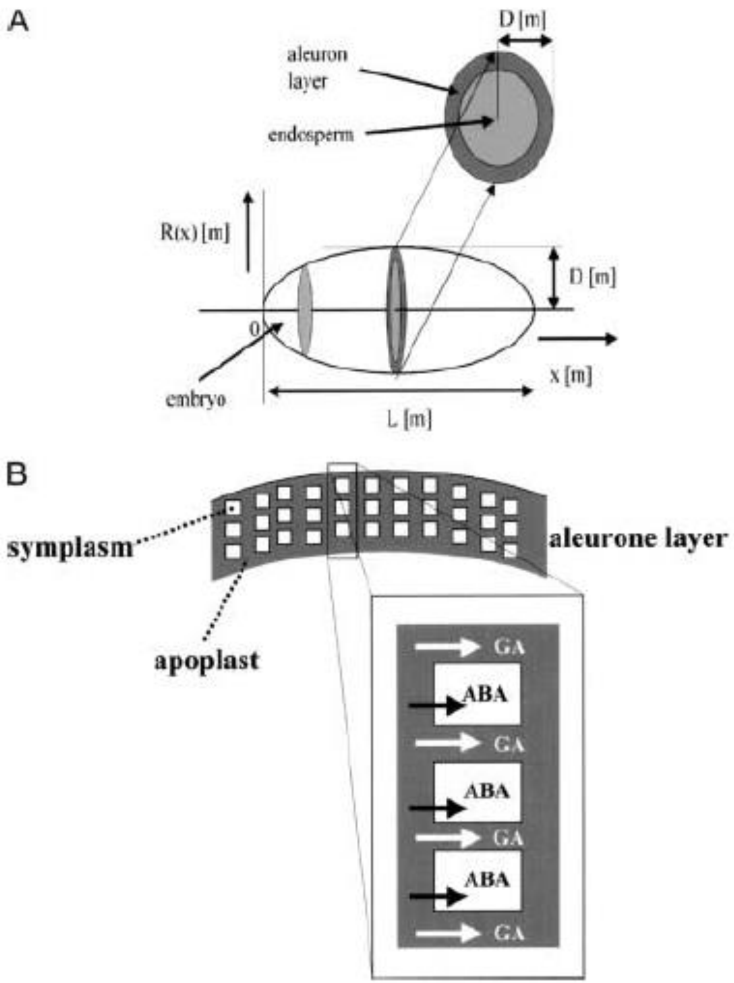


Fig. 4. Simulation model of wheat seed germination response to LDIR intensity variation.

Short notes on Mathematical models

ODE (and PDE) models



The diffusive transport of gibberellins and abscisic acid through the aleurone layer of germinating barley: a mathematical model.

Bruggeman, Libbenga and Van Duijn

Planta 2001, 214:89-96

Re-writing Eq. 14 and substituting Eq. 15, the mass balance for the diffusive transport of phytohormone through the apoplastic compartment is represented by Eq. 16.

$$\frac{\partial c_{apo}(x,t)}{\partial t} = \frac{D}{A_a(x) - n_{cell}(x) \cdot dc^2} \cdot \left(A_a(x) \cdot \frac{\partial^2 c_{apo}(x,t)}{\partial x^2} + \frac{\partial A(x)}{\partial x} \cdot \frac{\partial c_{apo}(x,t)}{\partial x} \right) - \frac{\phi_{pm}(x)}{V_{apo}(x)} \quad (16)$$

The mass balance for the cellular compartment results in Eq 17.

$$\frac{\partial c_{sym}(x,t)}{\partial t} = \frac{J_{pm}(x,t) \cdot A_{pm}(x)}{V_{sym}(x)} \quad (17)$$

Applying Fick's first law for the diffusion of the protonated form of the phytohormone and the Goldman equation (Lagarde 1976) for the electro-diffusive transport of the ionized form of the phytohormone, the total mass flux across the plasma membrane will be the superposition of the two fluxes, resulting in Eq. 20.

$$J_{pm} = J_{prot} + J_{ion} = D_{pm} \cdot \frac{c_{x,AH} - c_{x+d_{pm},AH}}{d_{pm}} + z \cdot F \cdot u \cdot \frac{\Delta\psi}{d_{pm}} \cdot \frac{c_{x+d_{pm},A^-} - c_{x,A^-} \cdot e^{\frac{-z \cdot F \cdot \Delta\psi}{R \cdot T}}}{e^{\frac{-z \cdot F \cdot \Delta\psi}{R \cdot T}} - 1} \quad (20)$$

Substituting Eqs. 18 and 19, the partition coefficient for the particular phytohormone form and Einstein's mobility relation in Eq. 20 results in an expression of the total mass flux $J_{pm}(x)$ as function of the concentration difference across the membrane.

$$J_{pm}(x) = \frac{D_{pm}}{d_{pm}} \cdot \left(K_{r,pro} \cdot \left[\frac{c_{apo}(x,t)}{1 + \frac{Ka}{H^+_{apo}}} - \frac{c_{sym}(x,t)}{1 + \frac{Ka}{H^+_{sym}}} \right] + \frac{z \cdot F}{R \cdot T} \cdot K_{r,ion} \cdot \Delta\psi \cdot \frac{\frac{c_{sym}(x,t)}{1 + \frac{H^+_{sym}}{Ka}} - \frac{c_{apo}(x,t) \cdot e^{\frac{-z \cdot F \cdot \Delta\psi}{R \cdot T}}}{1 + \frac{H^+_{apo}}{Ka}}}{e^{\frac{-z \cdot F \cdot \Delta\psi}{R \cdot T}} - 1} \right) \quad (21)$$

Short notes on Mathematical models

Statistical models

- Usually dealing with a pair (S and P), where S is the set of possible observations, i.e. the sample space, and P is a set of probability distributions on S.
- Model is non deterministic (variables can be stochastic, do not have a specific value).
- Used for Predictions, Information extraction, description of stochastic structures

A.I. and neuronal network models (specially in image analysis)

- Complex correlative models
- Using large numbers of parameters
- Using (very) large data sets

Mathematical Modelling in Seed Testing

- 13.30 Introduction to the initiative and types of modelling to consider

  Bert van Duijn, ATC / Tomoko Sakata, ATC
- 13.45 The Ellis-Roberts viability equations to model seed longevity in storage and extension into germination time courses via the PBT models

  Fiona Hay, MOI / Kent Bradford, ATC
- 14.10 A.I. Based Modelling in Seed Imaging Applications

  Kyle T. Peterson (Bayer Crop Sciences, Innovation Science & Engineering, USA)
- 14.45 Discussion on Assessing Uncertainty in Seed Testing Models & Statistics Committee Activities

  Jean-Louis Laffont, STA / Kirk Remund, STA
- 15.10 Wrap up and discussion.
- 15.25 Concluding remarks and brain refreshed departure

Thank you!

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