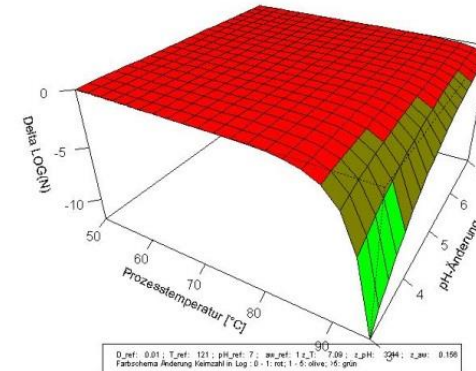
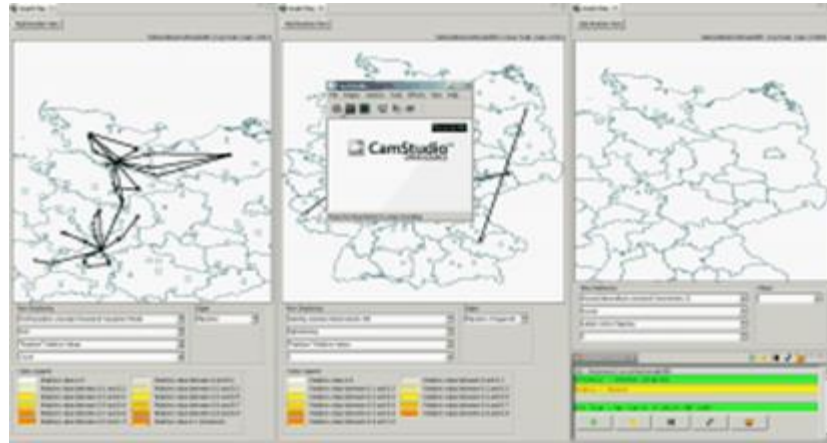


NextGen Food Safety Knowledge Integration Framework (initiative)

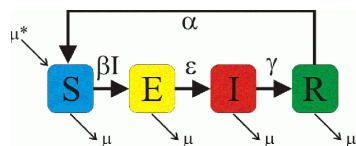
Matthias Filter (BfR)

A risk assessors "wish list"

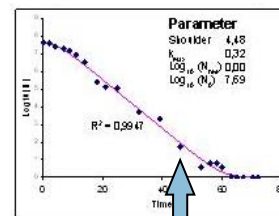
Ready-to-use mathematical models supporting (Ad-Hoc) risk assessments along the food chain



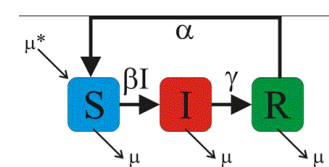
animal disease models



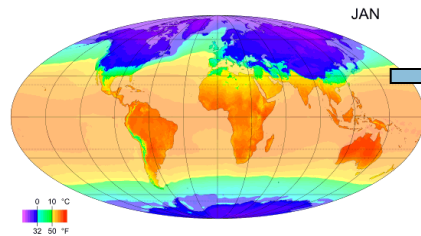
food processing and distribution



human disease models



Environmental factors



Processing parameters

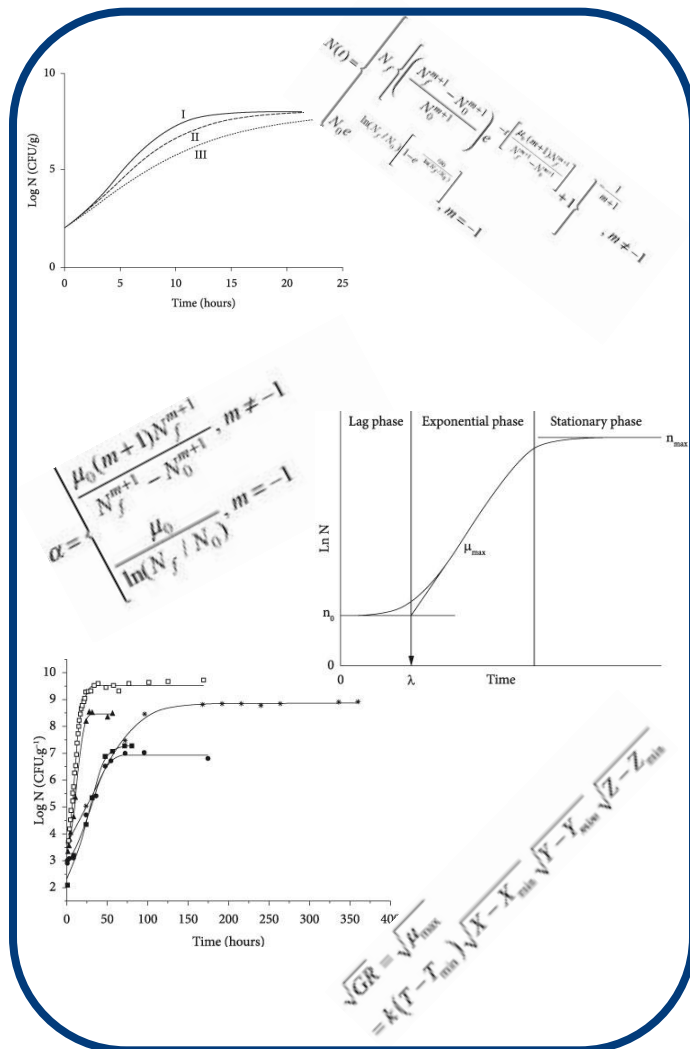


Current situation in the food safety modelling

1. Plenty of data and models published

2. Several software tools for model based predictions and simulations

3. However...



- NO common FORMAT to describe models / data
- => NO information exchange between software tools
- FEW open-source software solutions
- => FEW models implemented into ready-to-use tools
- => Re-use of EXISTING knowledge HAMPERED

Example: *Bacillus anthracis*



**(Ad-Hoc)
model-based
predictions
not possible!**

Literature:

✓ **Dozens** of papers containing **estimated models** of *B.anthraxis* in different food matrices (beef, milk, egg, etc.)

✓ **Dozens** of paper containing **data** on growth/inactivation of *B.anthraxis* in different food matrices and culture broth.

Predictive microbial software tools:

Estimated models available for predicting the growth or inactivation of *B.anthraxis*

1 (20-21 °C), (280-500 MPa)

Data records on growth/inactivation of *B.anthraxis*

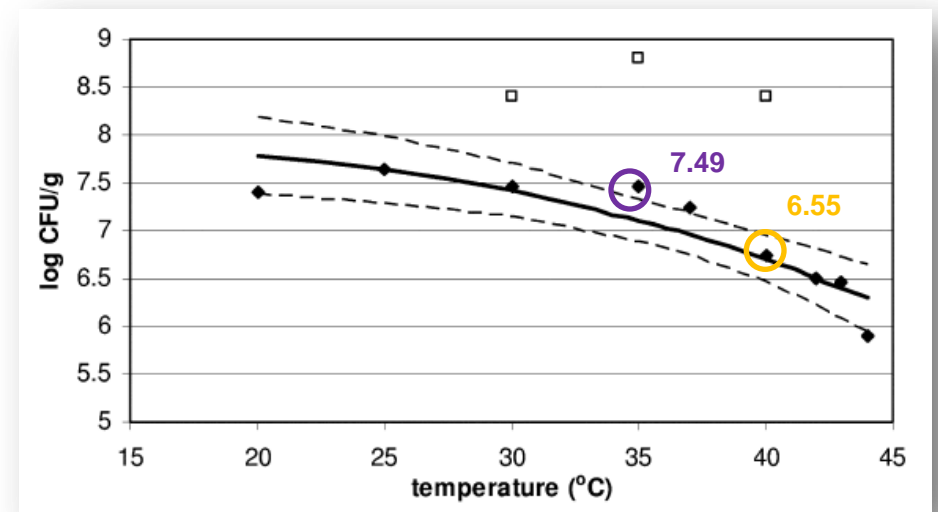
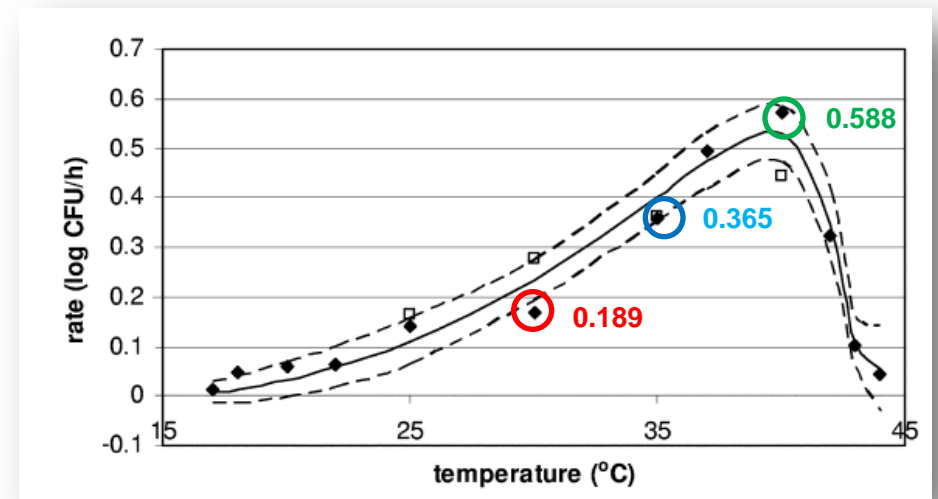
0

**Re-Implementation
of models
necessary !**

Issues with re-implementing estimated models

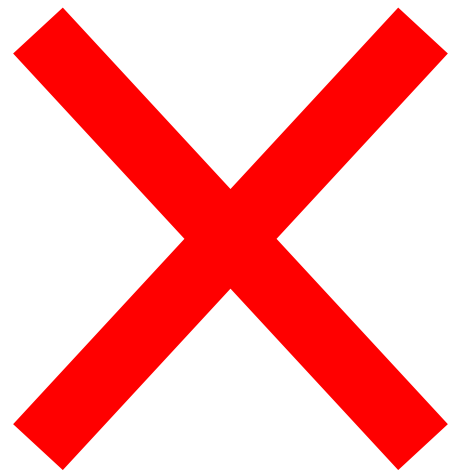
e.g. conflicting / wrong model parameters in papers

Temp (°C)	GR (log CFU/h)	LPD (h)	MPD (log CFU/g)
17	0.011 A	ND ^b	ND
18	0.049 B	52.6 A	ND
20	0.064 C	22.0 B	7.8 A
22	0.061 B	14.2 C	ND
25	0.153 (0.164) D	14.5 (15.5) C	7.7 (ND) A
30	0.221 (0.275) E	5.3 (6.3) D	7.8 (8.4) A
35	0.301 (0.362) F	6.2 (6.6) D	7.9 (8.8) A
37	0.496 G	3.5 D	7.3 A
40	0.488 (0.460) G	4.1 (3.7) D	7.3 (8.4) A
42	0.324 F	4.7 D	6.5 B
43	0.102 H	2.8 D	6.5 B
44	0.045 B	6.8 D	5.9 C



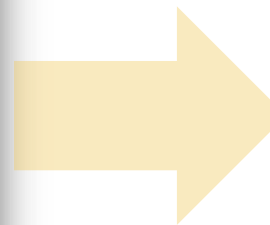
Issues when re-implementing estimated models

e.g. typos in model equations / formulas



$$LPD = a + b^{(-temp/c)}$$

(2)



$$LPD = a + b * \exp(-Temp/c)$$

Issues when re-implementing estimated models

e.g. erroneous re-implementation

Model Definition | Microbial Data | Flow Variables | Memory Policy

Model Properties

Model type: primary secondary primary (secondary)

Formula from DB: Juneja_2010_GroundBeef_BacillusAnthracic Refresh

Formula Name: Two Phase Linear Inactivation Model with intersect time-Juneja 2010 (v1429275346762) Type: inactivation/survival

Formula: $Value=Y0-(Time-Time_intersect)/D2*(Time>Time_intersect)-(Time/D1)+(Time-Time_intersect)/D1*(Time>Time_intersect)$ Apply

Boundary Conditions: Apply

Parameter	Unit	Independent	Value	...	Min	Max	Description
Value*	Number Content (count/mass) -> log10(count/g)	<input type="checkbox"/> Value			0.0	10.0	bacterial population at time t -log10() transformed
D1	Time -> min	<input type="checkbox"/>	0.088				D-value of first rate equation
D2	Time -> min	<input type="checkbox"/>	442.3				D-value of second rate equation
Time*	Time -> min	<input checked="" type="checkbox"/> Time			0.0	0.5	Time
Parameter Definition: Time_intersect	Time -> min	<input type="checkbox"/>	0.35				time point of intersection of two linear inactivation rate
Y0	Number Content (count/mass) -> log10(count/g)	<input type="checkbox"/>	7.0				initial bacterial population -log10() transformed

Model Name: Juneja_2010_GroundBeef_BacillusAnthracic

Goodness of fit: R²: RMS:
AIC: BIC:

Reference
Juneja, Vijay K. 2010_Thermal inactivation of Bacillus anthracis Sterne in irradiated ground beef heated in a water bath or cooked on commercial grills

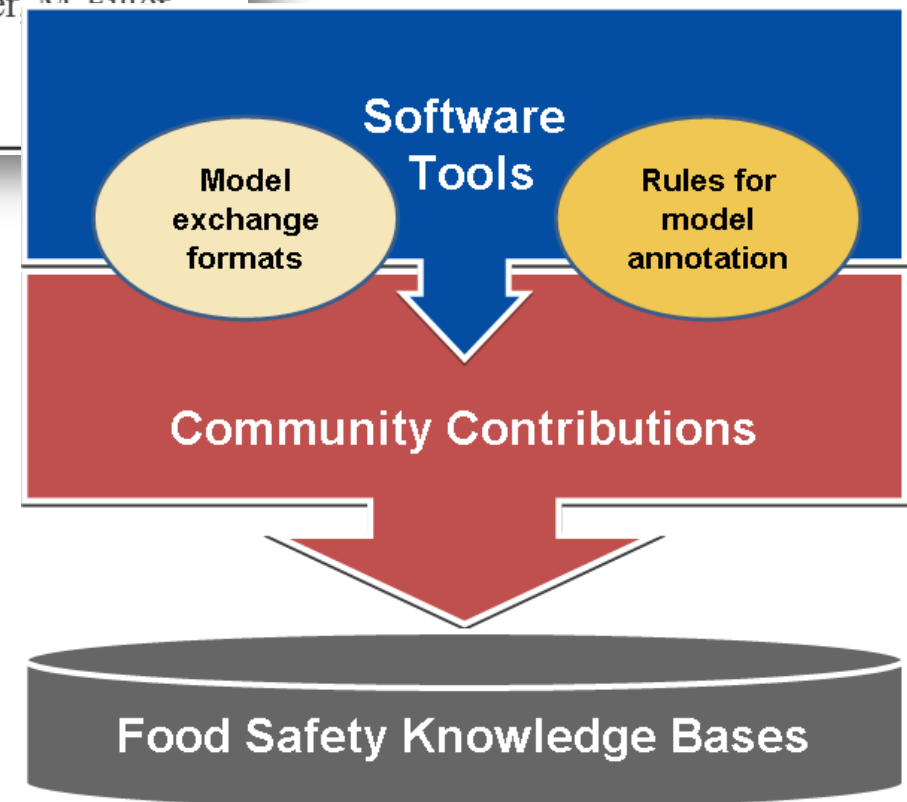
annotations

formulas

units

parameter values

Proposal



<http://www.researchgate.net/publication/273791203> A strategy to establish Food Safety Model Repositories

Details of proposed strategy

1. Establish a **standardized file format** (language) for estimated models (and experimental data)

→ interdisciplinary work of modellers and software engineers

2. Establish **rules for annotation** of models (and data)

→ agreement of scientists aiming to share estimated models

3. Enable **software tools to export / import** in this file format, e.g. *PMM-Lab*

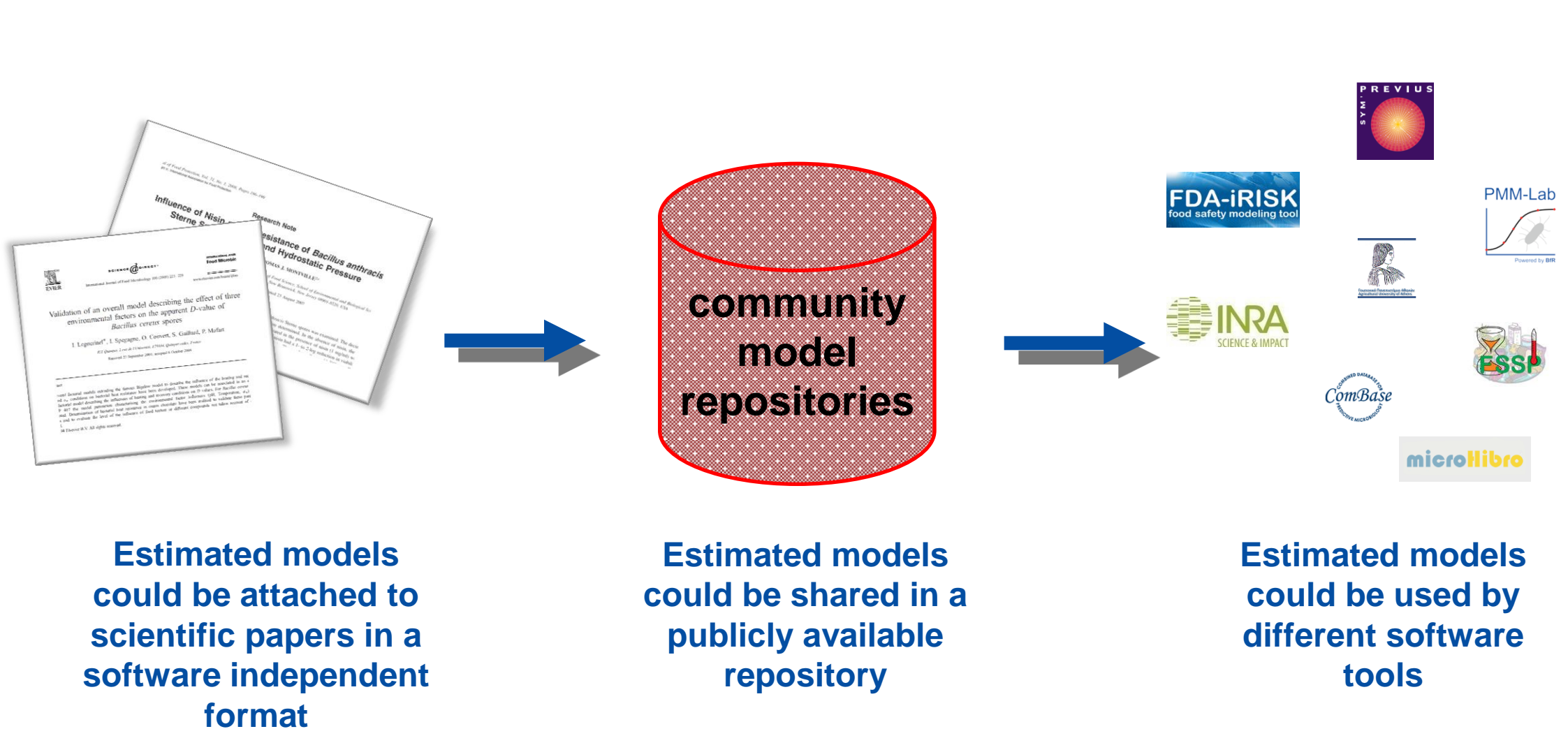
→ task of software engineers

→ Estimated models (and data) could easily be shared by those who create / re-implement them AND be validated / deployed by all others

Finally

Establish community driven Food Safety Model Repositories

to enable sharing of models (and data)



Current achievements

1.: Standardized file format: PMF-ML

Predictive Modelling in Food Markup Language

(PMF-ML)

Software Developer Guide

Version 1.1

Matthias Filter (Chair)	Federal Institute for Risk Assessment, Germany
Arvid Heise	Federal Institute for Risk Assessment, Germany
Christian Thöns	Federal Institute for Risk Assessment, Germany
Fernando Perez-Rodriguez	University of Cordoba, Spain
Miguel Ángel Cid García	Optimum Quality, Spain
Miguel de Alba Aparicio	Federal Institute for Risk Assessment, Germany

Contact:

Matthias Filter (matthias.filter@bfr.bund.de)

- ✓ Based on SBML v3
- ✓ Mathematical expressions encoded as MathML
- ✓ Meta data encoded using domain-specific controlled vocabularies

```
version="1.0" encoding="UTF-8" standalone="no"
Created by SBML Writer node version 1.0 on 2015-09-10 at 14:09:10 MEZ with JSBML version...

http://www.sbml.org/sbml/level3/version1/core
3
http://www.sbml.org/sbml/level3/version1/comp/version1
true
1

salm25
Three-Phase Linear Model (Buchanan et al., 1997) - iPMP Full Growth Models Eq 8 log10()...

culture_broth_broth_culture_culture_medium
true
culture broth, broth culture, culture medium

species4024
false
salmonella spp
false
log10_count_g
culture_broth_broth_culture_culture_medium

Time
false
0
h

k
true
0.014365402911347337
dimensionless
```

<http://sourceforge.net/projects/microbialmodelingexchange/>

2.: Rules for model annotation:

Learning from Systems Biology (MIRIAM Guidelines)

MANDATORY Information:

MIRIAM guidelines:

- Model name
- Model Identifier
- Creator(s)
- Creation date
- Rights
- Link to reference description
- Concordance between model and information in reference description

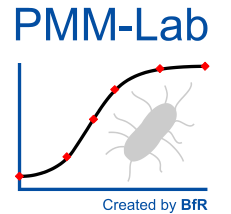
PMF specific extension:

- PMF-Organism (Microorganism(s))
- PMF-Environment (Food matrix)
- Range of applicability (environmental parameters, time, prediction values)

NON-COMPULSORY INFORMATION:

- Model's experimental raw data
- Goodness of fit
- Model uncertainties
- References to files containing data used for model generation or validation
- Range of application (e.g. other microorganisms / matrices)
- Experimental setup; details on food matrix and organisms.

3.: Software tools supporting PMF-ML PMM-Lab, (MicroHibro v2.0 Beta)



The screenshot displays the KNIME software interface with a workflow for PMF-ML. The workflow consists of five nodes:

- Model Reader**: Read Model from internal DB
- Primary Model Selection**: Look at model
- PMF Writer v2**: WRITE OUT as PMF-File
- PMF Reader v2**: READ IN any PMF-File
- Primary Model Selection**: Look at model

A red circle highlights the **PMF Writer v2** and **PMF Reader v2** nodes. Below the workflow, two dialog boxes for "Primary Model Selection" are shown, each displaying a graph of "Value (log10(count/g))" vs "Time [h]" and various configuration options.

4.: Community driven food safety model repository

The screenshot shows the open Food Safety Model Repository interface. At the top left is the logo and title: "open Food Safety Model Repository a community driven search engine for predictive microbial models". A search bar is on the top right. A left-hand menu contains options like "OPEN FSMR-DETAIL SEARCH VIEW". The main area features several filter dropdowns: "FullTextSearch", "PMF-Organism" (with "x Bacillus cereus" selected), "PMF-Environment", "Model-Type", "Model-DependentVariables", and "Software". Below the filters is a table of results with columns for "PMF-Organism", "PMF-Environment", "Model-Type", "Model-DependentVariables", and "Software". The first row is highlighted in yellow. To the right of the table is a "Details" pane with "Feature" and "Value" columns, showing information like "DOLU" date, "Model-Name", "PMF-Organism", etc. A "Übersetzt" button is at the bottom right of the details pane. Red arrows with numbers 1-5 point to specific features: 1. Software filter, 2. FullTextSearch input, 3. Download button in the menu, 4. OPEN FSMR-DETAIL menu option, and 5. Details pane.

- Core functionalities
1. Filter models according to predefined filter (e.g. Organism, Software etc.)
 2. Full-text search
 3. Download of result list
 4. Extended filter options via menu option: OPENFSMR-DETAIL
 5. Details on each model visible in the right pane

On the rise: software applications USING harmonized model files

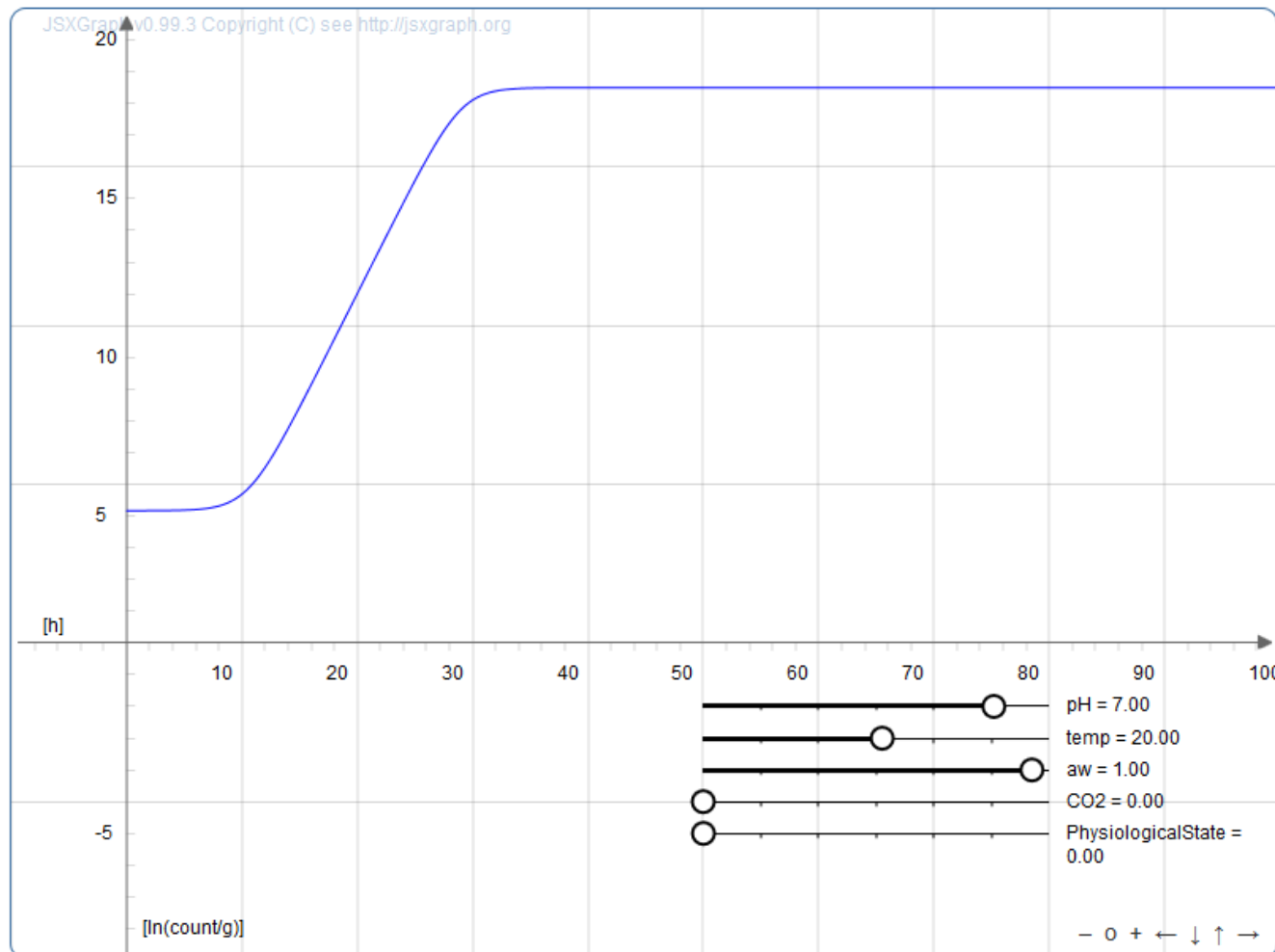
Model File

Change File

Uploaded file "Salmonella_GroundBeef_Temp-NaCl-SPP-NaL_InactivationSecondaryModel_Juneja2003_PMP.pmf" (2 KB)*



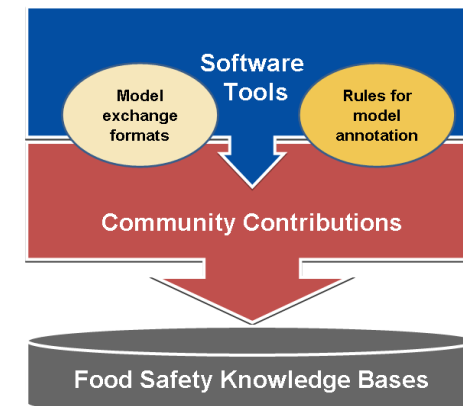
PMM Model Plot



Next Steps

- ❖ **Extend and improve FORMAT to describe models and simulations** (e.g. risk assessment models, dose response models, epidemiological models etc.)
- ❖ **Increase number of TOOLS SUPPORTING the FORMAT** (specifically existing modelling tools)
- ❖ **Advertise open MODEL REPOSITORIES** (including community contributions, curation)
- ❖ **Exploit models in decision support tools**

=> initiative needs funding



**Thanks to Laurent Guillier (ANSES)
and Maarten Nauta (DTU) supporting the
development of this joint initiative**

Thank you for your attention

Matthias Filter

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