

5/16/2009

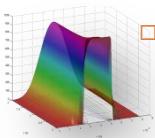
To be used with the EU-FP6 Project: MIGRESIVES
Author: olivier.vitrac@agroparistech.fr

ABOUT THE SFPP3 FRAMEWORK

It is meant preliminary for industrial users, which want to deploy easily mathematical migration modeling and last research results including decision tools for compliance testing and databases of physicochemical properties.

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- The SFPP3 framework is part of the effort at INRA to facilitate the distribution of industrial decision tools written in high-end mathematical language (C++, Matlab, Scilab...) without limiting third-party license restrictions and with minimal rewriting.
- By design the SFPP3 framework includes all capabilities broadly available on the Safe Food Packaging Portal version 2 (<http://h29.univ-reims.fr>), including multilayer migration modeling, advanced decision tools...
- Applications compatible with this framework, so-called SFPP3 applications, are available through a Web interface. As a result, they can be executed as standalone or remote applications, over a local area network or even over internet.
- As SFPP3 is HTML-centric, a new industrial application (which corresponds to a specific need) can be created by any web-designer with basic knowledge of HTML, CSS and Javascript (SPRY 1.6 Framework is implemented).
- The interface to large databases and computation engines (on server side) is provided using remote scripting (client side) with AJAX and XML, SOAP.
- SFPP3 is platform independent (tested on WIN32/64, Linux 32/64).
- **As templates, the current release of SFPP3 includes several fully functional applications: migration software (monolayer and multilayer), permeation software, 3D modeling...reporting tools (in Excel and PDF).**
- An enterprise-level application TOMATE (Tri-layer Optimized MATerial Engine) will be developed with SFPP3. As SFPP3 is completely extensible, the first step will consist in rewriting the web-interface (client side coding): diffusion_1DFVnx.sffp3.html to derive a simplified interface connected to a formulation database for polymers (first version is included in this package).
- By design, the SFPP3 framework complies with strong requirements of traceability. All inputs and outputs are uniquely stored and chronologically interrelated.
- Developing tools include: a debugging tool (to be incremented) to track misconfigurations and bugs, an automatic request builder for customized HTML and Javascript scripts.
- The distribution of SFPP3 is subjected to a license agreement with INRA (Institut National de la Recherche Agronomique, France).





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USER MANUAL

Here you will find an introduction of SFPP3 and a list of applications installed under the SFPP3 framework



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CONTENT FOR USERS

❖ SFFP3 PHILOSOPHY



❖ INSTALLATION



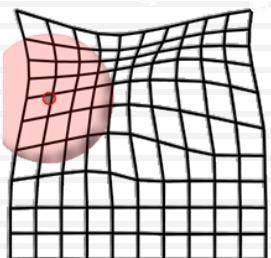
❖ AUTHENTIFICATION AND PROJECTS



❖ INSTALLED SFPP3 APPLICATIONS

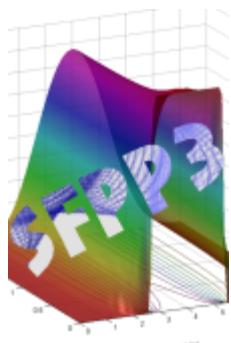
- ❖ NEW STANDARDS (SFPP3 ORIENTED)
- ❖ PREVIOUS APPLICATIONS (SFPP2 BASED)

❖ ADVANCED USER INTERFACE



(run-rich application)





PHILOSOPHY

SFPP3 = EXPANDABLE FRAMEWORK

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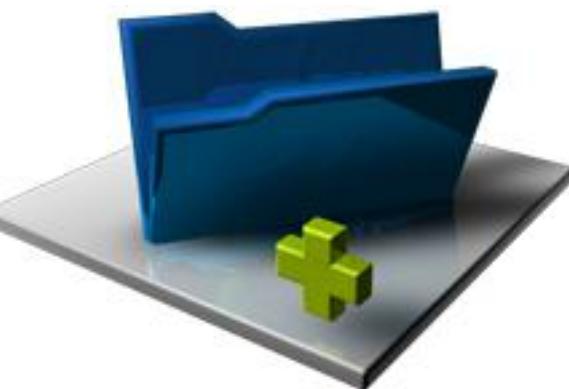
One server

One (default) or multiple clients

User authentication



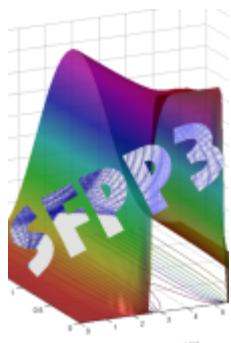
Efficient gateway enabling bidirectional connectivity between server-side components (simulation tools, 2D/3D plots, conversion tools...) and rich-client applications (using AJAX).



Powerful data management with shared and private projects.

Complete traceability of all actions (jobs submissions and individual results).

A unique data format = XML
Exported formats = XLS, PDF



ACCEPTED SERVER HOSTS

DEFAULT INSTALL = STANDALONE

6



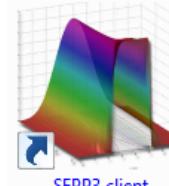
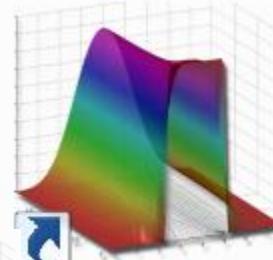
How to install:

C:\SFPP3\readme.txt
C:\SFPP3\install.bat
Restart your computer

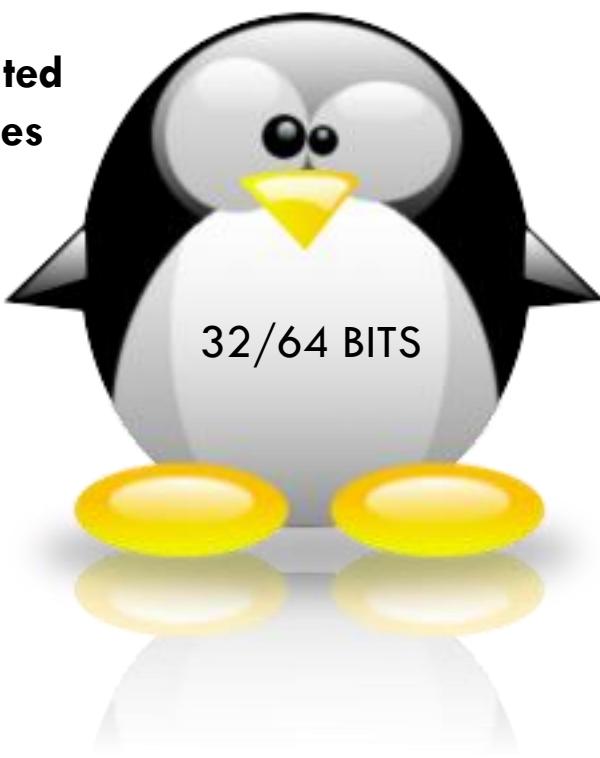


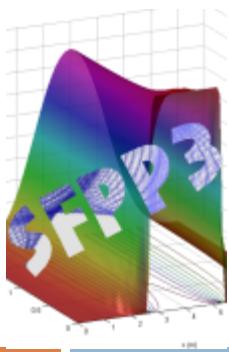
How to run:

Click on server icon
Click on client icon



The Linux install is not supported
in the EU-FP6 Project Migresives





RECOMMENDED BROWSERS (client-side)

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Javascript

- Fully compatible



Firefox® 3.1



Google Chrome





SFPP3: user-based access control to simulation tools and databases

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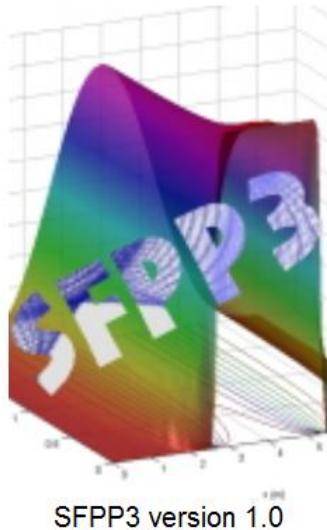
You have not logged in



[SFPP3 Login](#)

SFPP3: a framework to deploy migration simulation and decision tools
2009-02-03 11:36:18 unknown on WSLP-Olivier2(10.75.4.22)\MSWin32 <5.008007>
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac

SFPP3: login



Username: Olivier

Password: ······

SFPP3: a framework to deploy migration simulation and decision tools
2009-02-03 11:48:07 on WSLP-Olivier2(10.75.4.22)\MSWin32 <5.008007>
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac

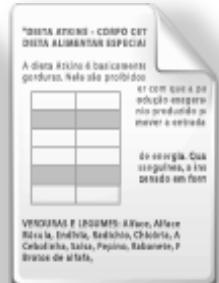


PROJECT SELECTOR

COLLABORATIVE AND PERSONAL PROJECTS

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A project = a collection of different simulation results



- [installed SFFP3 applications](#)
- [input files](#)
- [archives](#)
- [home/](#)
- [help](#)
- [»Logout«](#)
-

MY PROJECTS

user "Olivier" (change [user](#))

current project=common

(current database=common.sfpp3.database.xml)

| action | project | archive | description | |
|------------------------|------------------|-----------------------------|------------------------------------|---|
| select | common | common.sfpp3.database.xml | <i>project common to all users</i> |  |
| select | project 1 | project1.sfpp3.database.xml | <i>my project 1</i> |  |
| select | project 2 | project2.sfpp3.database.xml | <i>my project 2</i> |  |
| select | project 3 | project3.sfpp3.database.xml | <i>my project 3</i> |  |

SFPP3: a framework to deploy migration simulation and decision tools
 2009-02-05 08:53:08 Olivier on WSLP-Olivier2(10.18.3.100)\MSWin32 <5.008007>
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac



personal project



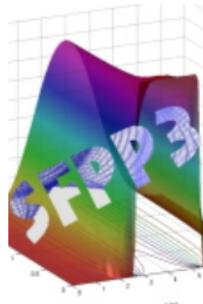
Project shared between several users



GETTING STARTED

LIST OF INSTALLED SFPP3 APPLICATIONS

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■ installed SFPP3 applications ■ input files ■ archives ■ home/ ■ map ■ help ■ debug ■ »Logout«

SFPP3 deployment server

Welcome Olivier ([change user](#))

2009-02-08 20:56:49



Getting started

You are accessing on your machine or on your local area network to applications, which have been developed for the online and academic version of the [SAFE FOOD PACKAGING PORTAL](#). SFPP3 hosts and executes reusable templates, databases, numerical codes to assess migration issues in food products. As SFPP3 is not subjected to third-party licenses, it can be used for commercial purposes as soon as you get an agreement with INRA (Institut National de la Recherche Agronomique). SFPP3 provides an inherent traceability of all actions and results (user-based and project-based identification). By changing the configuration file of SFPP3, it can be deployed to hundreds end-users. If you want to get more information on SFPP3 or if you want to deploy your own application on SFPP3 [click here](#).

You are working in the project: project 1 ([change project](#))

A project is collection of simulation data from one or several applications and shared or not between different users. The database corresponding to the current project is "[project1.sfpp3.database.xml](#)". You can access to simulation results associated to this project [here](#).

SFPP3 applications currently installed.

This page lists the different simulation tools of 1D mass transfer and their features available in this distribution of SFPP3. These tools can be used for compliance testing according to EU directive [2002/72/EC](#) and EU framework regulation [1935/2004/EC](#).

As SFPP3 is mainly HTML centric, a new application can be easily derived from an existing one or from scratch. Installed tools are focused on transport phenomena, including **diffusion, sorption, desorption, permeation**. The most appropriated term for "**migration**" of packaging constituents would be "diffusion-controlled desorption". All jobs submitted to this SFPP3 server are stored [here](#) as XML files for debugging and traceability purposes.

- Sort applications by name

- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications



SFFP3 APPLICATIONS WITH NEW USER INTERFACES

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APPLICATIONS

NEW STANDARDS

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Description:**Diffusion_1DFV2n.sfpp3.html** NEW

- Sort applications by name
- Diffusion_1DFV2n.sfpp3.html
- Adhesive
- Tomate
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Other applications

SFPP3 VERSION

New standard of rich-content SFPP3 application. This versatile application simulates the desorption from **multilayer** and **monolayer** materials (denoted P) in food or food simulants (denoted F).

P = multilayer and/or multimaterials consisting in up to 10 layers

F = liquid, semi-liquid (gel), solid.

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- **isotherm or anisotherm migration** NEW
- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- mass conservative numerical scheme
- very fast code
- **Accept templates and importation from previous simulations** NEW
- Calculates kinetics and profiles
- **Results from different simulations can be interactively compared** NEW
- **Mass balance effects can be explored in real time** NEW
- Results can be exported in **PDF and XLS**
- Fully compatible with last SFPP3 features (traceability, project management...).

The screenshot shows the SFPP3 software interface with the following details:

- My Information:** My user: demonever (Change user), My project: demonstration (Change project), My database: demo_sfpp3.database_and, My Application: Diffusion_1DFV2n (Change application). Date: 2009-03-26 08:00:27.
- Contact conditions:** A table with rows for U_F, V_F, A_F, dce_F, N_F, R, and t. Each row has input fields and an "import" button.
- Layer selector:** Shows "Layer 1" with properties: U_F (100), R_F (1), K_F/P (1), D_F (1e-10), Conc (0.001), and a "Layer 1" input field.
- Help:** Includes a note about unit conversion: "Unit value + 1000 ppm (except for plasticizers where 50% molar are required)".
- Buttons:** Save result as, Launch simulation.

APPLICATIONS

NEW STANDARDS

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- Sort applications by name

- Diffusion_1DFV2n.sfpp3.html
- Adhesive

■ SFPP3 applications ■ getting started ■ input files ■ archives ■ home/ ■ map ■ help ■ debug ■ »Logout« ■

My Information

My user: demouser ([change user](#))
 My project: demonstration ([change project](#))
 My database: demo.sfpp3.database.xml
 My Application: Diffusion_1DFV2n ([change application](#))

INRA\SFPP3 - 2009-03-28 09:44:40

PROJECT MANAGER

Archived simulations or templates

Trilayer
 Import properties from a previous result file in the current form

 Clear all properties in the current form

SEARCH TEMPLATES

Contact conditions

Layer selector

<< < > >>

Help

L_Fp: 50 kgF·kgP⁻¹
 V_F: µm³
 A_F: µm²
 rho_F: 1 kg·m⁻³ or g·cm⁻³
 k_F: 1
 Bi: 1000000
 t: 10 days
 Temperature :

Layer 1
 L_P: 80 µm
 rho_P: 1 kg·m⁻³ or g·cm⁻³
 K_F/P: 18
 D_P: 3.5e-013 m²·s⁻¹
 Conc.: 0 ppm

SELECTIVE IMPORT

Values of selected config:

L_Fp:160

rho:1

k:1

Bi:1000000

t:10 days

CONFIGURATION IN THE TEMPLATE

LAYERS:

L_P: [80 5 40] µm

rho: [1 1 1]

k: [18 0.2 1000]

D_P: [3.5e-013 1.1e-016 2.89e-016] m²·s⁻¹

C_P0: [0 1000 0] ppm

1D GEOMETRY APPROXIMATION

CUSTOMIZED NOMENCLATURE

Save result as:

Contact conditions

V_F: 300 cm³
 A_F: 150 cm²
 rho_F: 1 kg·m⁻³ or g·cm⁻³
 k_F: 1
 Bi: 1000000
 t: 10 days
 Temperature :

1D GEOMETRY APPROXIMATION

CUSTOMIZED NOMENCLATURE

Help

D_P

[SI unit: m²/s]

diffusion coefficient in P

CALCULATE OVERESTIMATES AND IMPORT IT

Use the form below as safe values (for the highest temperature).

Piringer Calculator

Polymer: PP (homo and random)

T: 40 °C

M: 200 g.mol⁻¹

APPLICATIONS

NEW STANDARDS

- Sort applications by name

- [Diffusion_1DFV2n.sfpp3.html](#)
- [Adhesive](#)

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Temperature : **set** **import**

My Information Archived simulations or templates

My user: demouser ([change user](#)) My project: demonstration ([change project](#))

My d My A INRA

Trilayer

SIMULATE HOT FILLING IN FEW CLICKS, CREATE TEMPLATES FOR TYPICAL PROBLEMS

Reset zoom Set temperature Cancel

| | start temperature | final temperature | duration | action |
|---|-------------------|-------------------|----------|------------------------------------|
| • | 20 °C | 80 °C | 10 sec | <input type="button" value="del"/> |
| • | 80 °C | 70 °C | 10 sec | <input type="button" value="del"/> |
| • | 70 °C | 60 °C | 20 sec | <input type="button" value="del"/> |
| • | 60 °C | 50 °C | 50 sec | <input type="button" value="del"/> |
| • | 50 °C | 30 °C | 2 min | <input type="button" value="del"/> |
| • | 30 °C | 25 °C | 2 min | <input type="button" value="del"/> |
| • | 25 °C | 20 °C | 5 min | <input type="button" value="del"/> |

Add step

My new result file Launch simulation

start temperature final temperature duration action

| | | | | |
|---|-------|-------|--------|------------------------------------|
| • | 20 °C | 80 °C | 10 sec | <input type="button" value="del"/> |
| • | 30 °C | 25 °C | 2 min | <input type="button" value="del"/> |
| • | 80 °C | 70 °C | 10 sec | <input type="button" value="del"/> |
| • | 70 °C | 60 °C | 20 sec | <input type="button" value="del"/> |
| • | 60 °C | 50 °C | 50 sec | <input type="button" value="del"/> |
| • | 50 °C | 30 °C | 2 min | <input type="button" value="del"/> |
| • | 25 °C | 20 °C | 5 min | <input type="button" value="del"/> |

Add step

SHIFT ANY SEGMENT TO A NEW POSITION

APPLICATIONS

NEW STANDARDS

- Sort applications by name

- Diffusion_1DFV2n.sfpp3.html**
- Adhesive

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Image results**Simulation report****kinetic graph****profile graph**

[SFPP3 applications](#) [getting started](#) [input files](#) [archives](#) [home/](#) [map](#) [help](#) [debug](#) [Logout](#)

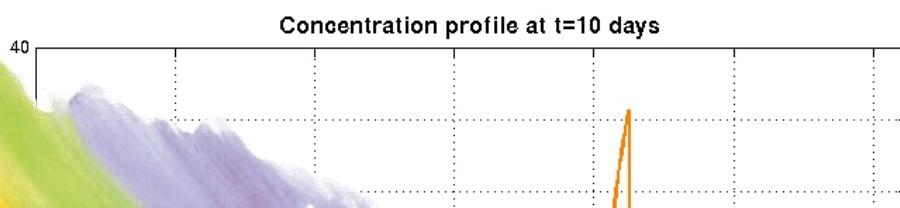
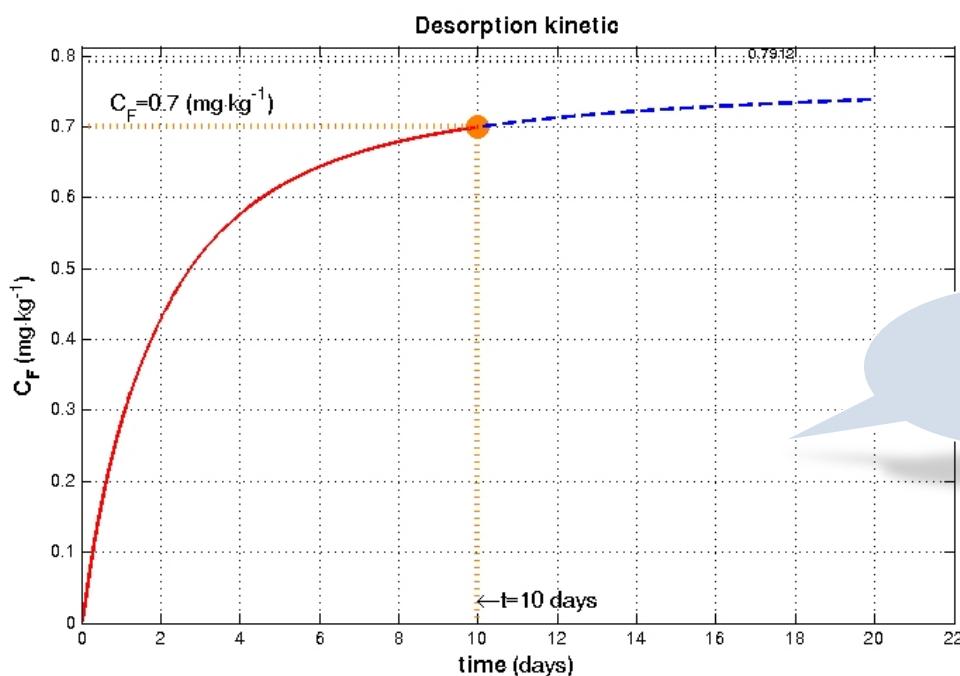
My Information

My user : **demouser** ([change user](#))
 My project : **Diffusion_1DFV2n** ([change project](#))
 My database : **demo.sfpp3.database**
 My Application : **demonstration** ([change application](#))

INRA\SFPP3 - 28-Mar-2009 09:28:56

Current simulation result

diffusion_1DFVn_18-Mar-2009_15-47-51_5180

[Rename](#) [Delete](#)[>>> EXCEL™ file <<<](#)[>>> PDF document <<<](#)[New simulation](#)
 EXPORT ALL
 NUMERICAL
 RESULTS
Image results**Simulation report****kinetic graph****profile graph**

APPLICATIONS

NEW STANDARDS

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- Sort applications by name
- [Diffusion_1DFV2n.sfpp3.html](#)
- Adhesive

[Image results](#)[Simulation report](#)[kinetic graph](#)[profile graph](#)

[SFPP3 applications](#) [getting started](#) [input files](#) [archives](#) [home/](#) [map](#) [help](#) [debug](#) [Logout](#)

My Information

My user : **demouser** ([change user](#))
 My project : **Diffusion_1DFV2n** ([change project](#))
 My database : **demo.sfpp3.database**
 My Application : **demonstration** ([change application](#))

INRA\SFPP3 - 28-Mar-2009 09:28:56

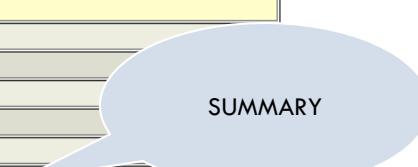
Current simulation result

diffusion_1DFVn_18-Mar-2009_15-47-51_5180

[Rename](#)[Delete](#)[>>> EXCEL™ file <<<](#)[>>> PDF document <<<](#)[New simulation](#)
EXPORT SUMMARY

[Image results](#)[Simulation report](#)[kinetic graph](#)[profile graph](#)

| Properties | Assigned values |
|--|--|
| ASSUMPTIONS | nlayers=3 1D desorption/one side contact (left) no swelling/plasticizing/blooming effects Henry isotherms |
| MESH QUALITY | normal |
| DILUTION FACTOR | $L_{FP}=50$ |
| GEOMETRIES | $L_P = [80 5 40] \mu m$ |
| DENSITIES | $\rho/\rho_0 = [1 1 1]$ |
| INITIAL CONCENTRATIONS | $C_{P0} = [0 1000 0] ppm$ |
| HENRY LIKE COEFFICIENTS | $k/k_0 = [18 0.2 1]$ |
| DIFFUSION COEFFICIENTS | $D_P = [3.5e-013 1.1e-016 2.89e-016] m^2.s^{-1}$ |
| DIMENSIONLESS EXTERNAL MASS TRANSPORT RESISTANCE | $Bi=h \cdot lref / Dref = 1e+006$ (reference layer = #3) |
| TIME/DIMENSIONLESS TIME | $t=10$ days; $Fo=Dref \cdot t / lref^2 = 0.1561$ (reference layer = #3) |
| REQUESTED CONCENTRATION IN FOOD OR SIMULANT | C_F=0.7 ppm |
| EXPECTED CONCENTRATION IN FOOD/SIMULANT AT EQUILIBRIUM | C_F_eq=0.791 ppm |
| time to reach 90% of C_F_eq | 12 days |
| time to reach 75% of C_F_eq | 4.4 days |
| time to reach 50% of C_F_eq | 1.7 days |
| time to reach 25% of C_F_eq | 15 hours |
| time to reach 10% of C_F_eq | 5.7 hours |
| time to reach 5% of C_F_eq | 3.2 hours |
| time to reach 1% of C_F_eq | 1.2 hours |
| time to reach 0.1% of C_F_eq | 35 minutes |
| SOLVER INFORMATION | CPU=4.78 s; solver="diffusion_1DFVn" host="127.0.0.1" |

SUMMARY


APPLICATIONS

NEW STANDARDS

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- Sort applications by name
- [Diffusion_1DFV2n.sfpp3.html](#)
- Adhesive

Image results Simulation report **kinetic graph** profile graph

SFPP3 applications getting started input files archives home/ map help debug [Logout](#)

My Information

My user : **demouser** ([change user](#))
 My project : **Diffusion_1DFV2n** ([change project](#))
 My database : **demo.sfpp3.database**
 My Application : **demonstration** ([change application](#))

INRA\SFPP3 - 28-Mar-2009 09:40:05

Current simulation result

diffusion_1DFVn_18-Mar-2009_15-47-51_5180

kinetic graph

Trilayer

Trilayer_Ab

Trilayer

Resolution: high average low

- Show cursors

COMPARE RESULTS FROM DIFFERENT SIMULATIONS

INTERACTIVE PLOTS WITH ZOOM, VALUES TRACKING

x = 3.32, y = 0.54

0.74
0.60
0.40
0.20
0.00

0.0 5.0 10.0 15.0 20.0

0 - 10 - 20

APPLICATIONS

NEW STANDARDS

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- Sort applications by name

- Diffusion_1DFV2n.sfpp3.html
- Adhesive

Image results**Simulation report****kinetic graph****profile graph**

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My Information

My user : demouser ([change user](#))
 My project : Diffusion_1DFV2n ([change project](#))
 My database : demo.sfpp3.database
 My Application : demonstration ([change application](#))

INRA\SFPP3 - 28-Mar-2009 09:40:05

Current simulation result

diffusion_1DFFn_18-Mar-2009_15-47-51_5180

[Rename](#)[Delete](#)

>>> EXCEL™ file <<<

>>> PDF document <<<

[New simulation](#)**Image results****Simulation report****kinetic graph****profile graph**

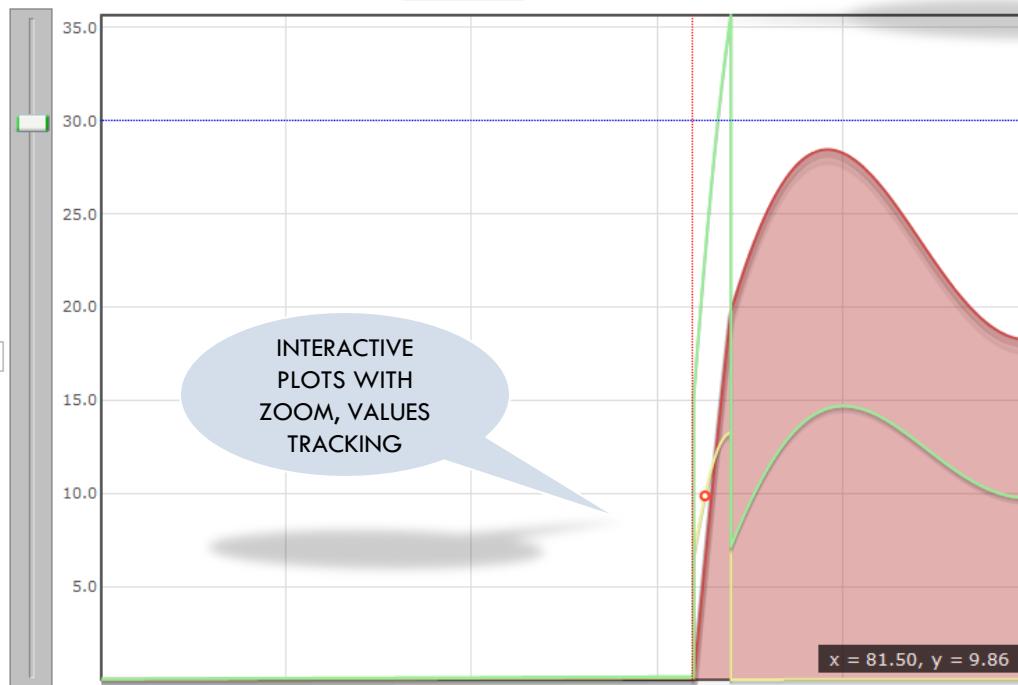
Trilayer

Trilayer_Ab [delete](#)Trilayer [delete](#)[Reset zoom](#) - Show cursors

COMPARE
RESULTS FROM
DIFFERENT
SIMULATIONS

INTERACTIVE
PLOTS WITH
ZOOM, VALUES
TRACKING

x = 81.50, y = 9.86



APPLICATIONS

Migration from adhesives

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- Sort applications by name
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

Adhesive.sfpp3.html

SFPP3 VERSION

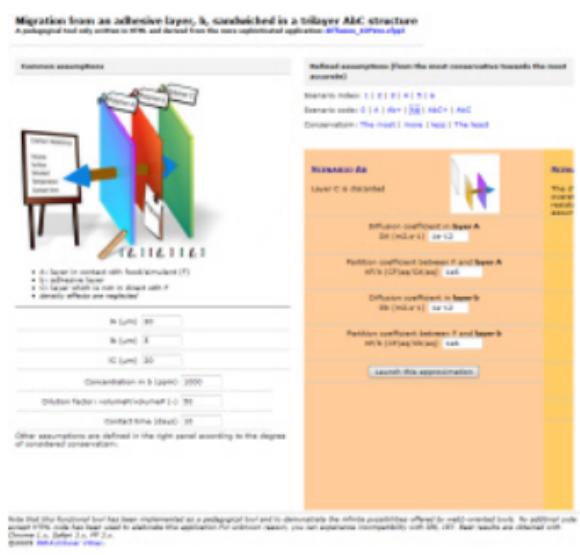
A **pedagogical and functional tool** to illustrate how iterative modeling can be used to handle uncertainty in the demonstration of the compliance of **adhesives** used in food packaging applications.

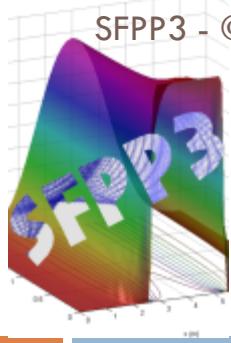
The plastic material, P, is coded AbC, where b is the adhesive layer, A is the polymer layer in contact with F, C is a polymer layer which is not in direct contact with F
 F = liquid, semi-liquid (gel), solid food or food simulant

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- **iterative modeling**
- possible external mass transfer resistances are considered
- finite volume effects are considered
- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- mass conservative numerical scheme
- very fast code
- the numerical accuracy can be controlled by the user
- Calculates kinetics in F and profiles in P
- Results can be exported in **PDF and XLS**
- Connection to databases requires the web version





APPLICATIONS MIGRATION FROM ADHESIVES

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- Sort applications by name
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

TOMATE = Trilayer Optimized MATerials Engine

An **expert system** including a simulation engine, large databases of adhesive formulations and physical properties to demonstrate the compliance of **adhesives** used in food packaging applications

This application is currently on development in the FP6 European Project [Migresives](#).

Features:

- an interactive interface for inputs and outputs
- formulation databases
- databases diffusion coefficient for polyolefins
- databases of activity coefficients calculated from molecular simulations
- an automatic scenario generator



layer material - Mozilla Firefox

que Marque-pages Outils ?

http://localhost/home/Diffusion_1DFV2n.sfpp3.html

SFPP3 applications getting started input files archives home/ map help debug »Logout»

My Information

User ([change user](#))
non ([change project](#))
common.sfpp3.database.xml
diffusion_1DFV2n ([change application](#))

09-05-04 21:05:33

Archived simulations or templates

Select a simulation result or a template

Import properties from a previous result file in the current form

geometry **formulation** **contact conditions** **transport**

Import properties from a previous result file as concentration profile

Concentration profile

Clear all properties in the current form

form reset

Search migrant in database : MigrantsDB propertiesDB
by chemical name

Layer selector

<< < > >> 3

Help

conditions

kgF/kgP⁻¹ import
cm³ import
cm² import
kg·m⁻³ or g·cm⁻³ import
m² import
days import
set import

Layer 1

| | | |
|-------|--|----------|
| I_P | μm | import |
| rho_P | kg·m ⁻³ or g·cm ⁻³ | import |
| K_F/P | 1 | import T |
| D_P | 1e-14 m ² s ⁻¹ | import T |
| Conc. | ppm | import |

This area will display information and help

For any question, send an e-mail to [Olivier Vitrac](#)

All results are provided AS IS.

Launch simulation

Acceptable threshold or specific migration limit : ppm

SFPP3: a framework to deploy migration simulation and decision tools
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac
 Design by [Soprogix](#)

21

DIFFUSION_1DFV2N.SFPP3.HTML

SHORT MANUAL

A COMMON INTERFACE FOR TOMATE AND MULTILAYER APPLICATIONS (DESORPTION APPLICATIONS)



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

22

PRINCIPLES: 6 MAIN AREAS

QSPR:: Diffusion Simulation - multilayer material - Mozilla Firefox

Eichier Édition Affichage Historique Marque-pages Outils ?

http://localhost/home/Diffusion_1DFV2n.sfpp3.html

SFPP3 applications getting started input files archives home/ map help debug >Logout<

My Information

My user: demouser ([change user](#))
 My project: common ([change project](#))
 My database: common.sfpp3.database.xml
 My Application: Diffusion_1DFV2n ([change application](#))

INRA\SFPP3 - 2009-05-04 21:05:33

Archived simulations or templates

Select a simulation result or a template
 Import properties from a previous result file in the current form
 geometry formulation contact conditions transport prop. all
 Import properties from a previous result file as concentration profile
 Concentration profile
 Clear all properties in the current form
 form reset

Search migrant in database : MigrantsDB propertiesDB
 by chemical name

Contact conditions

L_FP 50 kgF·kgP⁻¹ import
 V_F cm³ import
 A_F cm² import
 rho_F 1 kg·m⁻³ or g·cm⁻³ import
 k_F 1 import
 Bi 1e6 import
 t 0 days import
 Temperature : [set](#) import

Layer selector

<< < > >> 3

Layer 1

I_P µm import
 rho_P 1 kg·m⁻³ or g·cm⁻³ import
 K_F/P 1 import T
 D_P 1e-14 m²·s⁻¹ import T
 Conc. ppm import

Help

This area will display information and help.
 For any question, send an e-mail to [Olivier Vitrac](#).

All results are provided AS IS.

Save result as:
[Summary](#) [Launch simulation](#)

Acceptable threshold or specific migration limit : ppm

SFPP3: a framework to deploy migration simulation and decision tools
 SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac
 Design by [Soprogix](#)

1 Project information

2 Previous results, templates, databases

3 Definition of contact conditions

4 Material definition

5 Help area, database details and additional information

6 Traceability and decision making area



DIFFUSION_1DFV2N.SFPP3.HTML INTERACTIVE INPUT FORM

23

PRINCIPLES: 6 MAIN AREAS

My Information

1

My user: **demouser** ([change user](#))

My project: **common** ([change project](#))

My database: **common.sfpp3.database.xml**

My Application: **Diffusion_1DFV2n** ([change application](#))

[INRA\SFPP3](#) - 2009-05-04 21:05:33

User = current user as authentified

Project = specific area (repository) where results are virtually stored and possibly shared between users

Database = index that lists results belonging to a given project

Application = HTML document that setups the user interface (a new SFPP3 application is created by adding a new HTML document)





DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

24

PRINCIPLES: 6 MAIN AREAS

diffusion_1DVFn_24-Mar-2009_16-03-40_1090

Import properties from a previous result file in the current form

geometry

formulation

contact conditions

transport prop.

all

Import properties from a previous result file as concentration profile

Concentration profile

Clear all properties in the current form

form reset

Search migrant in database : MigrantsDB propertiesDB

by chemical name

2

diffusion_1DVFn_24-Mar-2009_16-03-40_1090

Select a simulation result or a template

- activation 2
- activation
- debug3
- debug3
- debug2
- debug1
- debug1
- debug1
- debug1
- diffusion_1DVF
- diffusion_1DVF
- diffusion_1DVF
- toto3
- toto2
- toto
- diffusion_1DVFn_27-Apr-2009_09-39-32_9710
- diffusion_1DVFn_26-Apr-2009_11-21-06_8320



**PREVIEW OF
PREVIOUS SIMULATIONS
OR TEMPLATES**
(here a trilayer)

Help

Selected configuration

L_FP:50
rho:1
k:1
Bi:1000
t:10 days

Contact
conditions

LAYERS:

I_P: [30 5 20] µm
rho: [1 1 1]
k: [1000000 1000000 1000000]
D_P: [1e-012 1e-012 1e-009] m².s⁻¹
C_PO: [0 1000 0] ppm

Layers
properties

5



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

25

PRINCIPLES: 6 MAIN AREAS

diffusion_1DVFn_24-Mar-2009_16-03-40_1090

Import properties from a previous result file in the current form

geometry **formulation** **contact conditions** **transport prop.** **all**

Import properties from a previous result file as concentration profile

Concentration profile

Clear all properties in the current form

form reset

Search migrant in database : MigrantsDB propertiesDB

by chemical name

2

SELECTIVE IMPORT FROM SIMULATIONS
OR TEMPLATES



Contact conditions

| | | | |
|---|----------------------|---|---------------------------------------|
| <input checked="" type="radio"/> L_FP | 50 | kgF·kgP ⁻¹ | <input type="button" value="import"/> |
| <input type="radio"/> V_F | <input type="text"/> | cm ³ | <input type="button" value="import"/> |
| <input type="radio"/> A_F | <input type="text"/> | cm ² | <input type="button" value="import"/> |
| rho_F | 1 | kg·m ⁻³ or g·cm ⁻³ | <input type="button" value="import"/> |
| k_F | 1 | | <input type="button" value="import"/> |
| Bi | 1000 | | <input type="button" value="import"/> |
| t | 10 | days | <input type="button" value="import"/> |
| <input type="checkbox"/> Temperature : <input type="button" value="set"/> <input type="button" value="import"/> | | | |



DIFFUSION_1DFV2N.SFPP3.HTML INTERACTIVE INPUT FORM

26

PRINCIPLES: 6 MAIN AREAS

Archived simulations or templates

diffusion_1DVFn_24-Mar-2009_16-03-40_1090 ▾
Import properties from a previous result file in the current form
geometry **formulation** **contact conditions** **transport prop.** **all**
Import properties from a previous result file as concentration profile
Concentration profile **activation**
Clear all properties in the current form
form reset
Search migrant in database : MigrantsDB propertiesDB
by chemical name ▾



Start a simulation with a previously calculated concentration profile (here *from simulation so-called “activation”*) as initial concentration profile (e.g. to simulate the setoff effect).

Layer geometries must be compatible



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

27

PRINCIPLES: 6 MAIN AREAS

Archived simulations or templates

diffusion_1DVFn_24-Mar-2009_16-03-40_1090

Import properties from a previous result file in the current form

geometry

formulation

contact conditions

transport prop.

all

Import properties from a previous result file as concentration profile

Concentration profile

Clear all properties in the current form

form reset

Search migrants/data: Migrants (M,SML...) Transport Properties

name/IUPAC ▾ irganox 1076

octadecyl 3-(4-hydroxy-3,5-ditert-butyl-phenyl)propanoate



2



Database of migrants includes:

- >3300 substances,
- >25000 synonyms
- >3200 CAS numbers,
- >2000 PMREF codes

Intelligent search so that a commercial/common name leads to its IUPAC name (when available)

Search migrants/data: Migrants (M,SML...) Transport Properties

name/IUPAC ▾ bht

Butylated hydroxytoluene

Search migrants/data: Migrants (M,SML...) Transport Properties

name/IUPAC ▾ irgafos 168

tris(2,4-ditert-butylphenoxy)phosphane



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

28

PRINCIPLES: 6 MAIN AREAS

Search migrants/data

INTELLIGENT SEARCH



Search migrants/data: Migrants (M,SML...) Transport Properties

CAS number

769-78-8
121-69-7
693-23-2
106-69-4
26952-21-6
694-91-7
691-37-2
6996-01-6
92-69-3
25322-69-4
69-72-7
26914-43-2
90021-69-5
100-69-6
085711-69-9



2

Search migrants/data: Migrants (M,SML...) Transport Properties

formula

C33H50O6P2
C33H39N3O2
C33H56N4OS2
C33H66O
C33H59NO4
C33H64O6
C33H47NO13
C33H54O6



2



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

29

PRINCIPLES: 6 MAIN AREAS

Search migrant in database : MigrantsDB propertiesDB
by chemical name ▼ 1,3-Benzenedicarboxylic acid

2

REGULATION DATA
AND OTHER
RELEVANT DATA

AUTOFILLING OF
FORMS



Migrant found: 1,3-Benzenedicarboxylic acid

Name: [1,3-Benzenedicarboxylic acid \(Isophthalic acid; m-Benzenedicarboxylic acid; m-Phtalic acid; Benzene,1,3-dicarboxylic acid; Acide isop...\)](#)

CAS: [121-91-5](#)

REF: 19150

Formula: C₈H₆O₄

M: 166.1308 g/mol

SML: 5 ppm

EFSA: R = 5 mg/kg of food. Available: Migration data, 7 mutagenicity studies regarded as non-genotoxic, 28-day inhalation and 90-day oral rat studies, inhalation rat teratology study limited absorption and excretion data (RIVM/TNO SDS CS/PM/2757, January 96).

EU Regulation: +Positive List

SCF opinion=substance with TDI=tolerable daily intake

5

Acceptable threshold or
specific migration limit :

5

ppm



6

Piringer Calculator

| | | |
|----------|----------|---------------------|
| Polymer: | LDPE | °C |
| T: | 40 | g.mol ⁻¹ |
| M: | 166.1308 | |

M of 1,3-Benzenedicarboxylic acid: **166.1308**

Import in current layer





DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

30

PRINCIPLES: 6 MAIN AREAS

Help

Migrant found: 1,3-Benzenedicarboxylic acid

Name: [1,3-Benzenedicarboxylic acid](#) (Isophthalic acid; m-Benzenedicarboxylic acid; m-Phtalic acid; Benzene,1,3-dicarboxylic acid; Acide isop...)

CAS: [121-91-5](#)

REF: 19150

Formula: C₈H₆O₄

M: 166.1308 g/mol

SML: 5 ppm

EFSA: R = 5 mg/kg of food. Available: Migration data, 7 mutagenicity studies regarded as non-genotoxic, 28-day inhalation and 90-day oral studies, inhalation rat teratology study limited absorption and excretion data (RIVM/TNO SDS CS/PM/2757, January 96).

EU Regulation: +Positive List

SCF opinion=substance with TDI=tolerable daily intake

5

PREVIEW OF
>1500 SUBSTANCES

1,3-Benzenedicarboxylic acid Close

InChI=1S/C₈H₆O₄/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H, (H,9,10)(H,11,12)
Hash: QQVIHTCHCMHWDBS-UHFFFAOYSA-N

Toxicity [EPA DSSTox](#) [autosearch](#)



DIFFUSION_1DFV2N.SFPP3.HTML

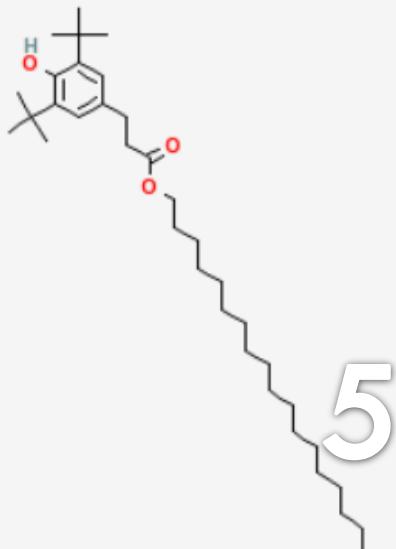
INTERACTIVE INPUT FORM

31

PRINCIPLES: 6 MAIN AREAS

octadecyl 3-(4-hydroxy-3,5-ditert-butyl-phenyl)propanoate

Close



PREVIEW OF
>1500 SUBSTANCES

LINK TO
TOXICOLOGICAL
DATA



InChI=1S/C35H62O3
/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-38-32(36)25-24-29-27-30(34(2,3)4)33(37)31(28-29)35(5,6)7
/h27-28,37H,8-26H2,1-7H3
Hash: SSDSCDGVMJFTEQ-UHFFFAOYSA-N

Toxicity

EPA DSSTox

[autosearch](#)

EXTERNAL LINKS



| Query | Results Type | Hits | Display |
|---|--------------|------|-------------------------|
| InChI: InChI=1S/C35H62O3/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-38-32(36)25-24-29-27-30(34(2,3)4)33(37)31(28-29)35(5,6)7 /h27-28,37H,8-26H2,1-7H3 | Matches | 1 | Details |
| | | | |

EPA DSSTox
Structure-Browser v2.0

Search

File Incidences

Search

DSSTox Chemical Text Search

Choose search: Auto-detect

[Clear](#) [Search](#)



| DSSTox ID | Similarity Score% | Structure Match | Substance Name | CASRN | Substance Description | Details (Data Files) | |
|-----------|-------------------|--|---|-----------|--------------------------|----------------------|--------|
| | | | | | | HPVCSI | HPVISD |
| 27456 | 100 | CH ₃ -~~~O(CH ₂) ₃ OH(CH ₃) ₂ | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl-ester | 2082-79-3 | single chemical compound | KIERBL | HPVISD |

| | |
|----------------------------|---|
| DSSTox RID | 39391 |
| DSSTox_Generic_SID | 27456 |
| TestSubstance_ChemicalName | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl-ester |
| TestSubstance_CASRN | 2082-79-3 |
| TestSubstance_Description | single chemical compound |
| STRUCTURE_Shown | tested chemical |
| StudyType | Receptor Binding |
| Endpoint | Estrogen receptor competitive binding: I |
| Species | rat |
| Source_ChemicalName | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl-ester |
| Assay_Target | Rat uterine cytosol (RUC) estrogen receptor binding |
| ActivityOutcome_KIERBL | inactive |
| ActivityScore_KIERBL | 0 |
| BindingCurve_Group | None |



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

32

PRINCIPLES: 6 MAIN AREAS

EXTERNAL LINKS



Help

Migrant found: 1,3-Benzenedicarboxylic acid

Name: 1,3-Benzenedicarboxylic acid (isophthalic acid; m-Benzenedicarboxylic acid; m-Phthalic acid; Benzene,1,3-dicarboxylic acid; Acide isop...)

CAS: 121-91-5

REF: 19150

Formula: C₈H₆O₄

M: 166.1308 g/mol

SML: 5 ppm

EFSA: R = 5 mg/kg of food. Available: Migration data, 7 mutagenicity studies regarded as non-genotoxic, 28-day inhalation and 90-day oral rat studies, inhalation rat teratology study limited absorption and excretion data (RIVM/TNO SDS CS/PM/2757, January 96).

EU Regulation: +Positive List
SCF opinion= substance with TDI=tolerable daily intake

5

Drug and Chemical Information: (Total:1) [?](#)

isophthalate

Safety and Toxicology [?](#)

HSDB - Peer-reviewed summary of toxicity and biomedical effects

NIOSH ICSC - NIOSH International Chemical Safety Cards

CCCRIS - Carcinogenicity, tumor promotion, tumor inhibition, and mutagenicity tests

EINECS - European Inventory of Existing Commercial Chemical Substances

TOXLINE - Citations to the toxicological literature



Literature

Literature Keyword Mining Tool [?](#)

Properties Computed from Structure: [?](#)

| | |
|-----------------------------------|--|
| Molecular Weight | 166.13084 [g/mol] |
| Molecular Formula | C ₈ H ₆ O ₄ |
| XLogP3 | 1.7 |
| H-Bond Donor | 2 |
| H-Bond Acceptor | 4 |
| Rotatable Bond Count | 2 |
| Exact Mass | 166.026609 |
| MonoIsotopic Mass | 166.026609 |
| Topological Polar Surface Area | 74.6 |
| Heavy Atom Count | 12 |
| Formal Charge | 0 |
| Complexity | 179 |
| Isotope Atom Count | 0 |
| Defined Atom StereoCenter Count | 0 |
| Undefined Atom StereoCenter Count | 0 |
| Defined Bond StereoCenter Count | 0 |
| Undefined Bond StereoCenter Count | 0 |
| Covalently-Bonded Unit Count | 1 |

Descriptors Computed from Structure: [?](#)

IUPAC Name: benzene-1,3-dicarboxylic acid
 Canonical SMILES: Cl=C(C=C(Cl)C(=O)O)C(=O)O
 InChI: InChI=1S/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)1
 InChIKey: QQVIIHTCMHWDBS-UHFFFAOYSA-N

Compound Information: [?](#)

CID 8496 [?](#) [?](#)
 Create Date: 2004-09-16

Related Compounds: [?](#)
 Same, Connectivity: 3 Links

Similar Compounds: 540 Links [?](#)
 Similar Conformers: 2387 Links [?](#) View Conformers [?](#)

Substance Information: [?](#)

Substances: [?](#)
 All: 651 Links
 Same structure: 43 Links
 Mixture: 608 Links

Category: [for same structure substances] [?](#)
 Biological Properties: 7 Links
 ChEBI (1)
 SID 8147985 - External ID: CHEBI:30802
 DiscoveryGate (1)
 SID 8156000 - External ID: 8496
 DTP/NCI (1)
 SID 79219 - External ID: 15310
 LeadScope (1)
 SID 49986259 - External ID: LS-85233
 NextBio (1)
 SID 50608838 - External ID: 8496
 NIAID (1)
 SID 607564 - External ID: 018124
 NovoSeek (1)
 SID 57325056 - External ID: 8496

Journal Publishers: 1 Link
 Thomson Pharma (1)
 SID 15120377 - External ID: 00061640

NIH Molecular Libraries: 1 Link
 NCGC (1)
 SID 26757427 - External ID: NCGC00164010-01



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

33

PRINCIPLES: 6 MAIN AREAS

EXTERNAL LINKS



National Institute of Standards and Technology

Help

Migrant found: 1,3-Benzenedicarboxylic acid

Name: [1,3-Benzenedicarboxylic acid](#) (*Isophthalic acid; m-Benzenedicarboxylic acid; m-Phthalic acid; Benzene, 1,3-dicarboxylic acid; Acide isop...*)

CAS: [121-91-5](#)

REF: 19150

Formula: C₈H₆O₄

M: 166.1308 g/mol

SML: 5 ppm

EFSA: R = 5 mg/kg of food. Available: data, 7 mutagenicity studies regarded as non-genotoxic, 28-day inhalation and 90-day studies, inhalation rat teratology study, absorption and excretion data (RIVM/TNO CS/PM/2757, January 96).

EU Regulation: +Positive List
SCF opinion= substance with TDI=tolerable intake

5

1,3-Benzenedicarboxylic acid

- **Formule:** C₈H₆O₄
- **Poids moléculaire:** 166.1308
- **Identifiant Chimique Internationale IUPAC:**
 - InChI=1S/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H, (H, 9, 10)
 - Télécharger l'identifiant dans un fichier.
- **IUPAC InChIKey:** QQVIHTCMHWDBS-UHFFFAOYSA-N
- **Numéro d'enregistrement CAS:** 121-91-5
- **Structure Chimique:**

O=C(Oc1ccc(C(=O)O)cc1)C(=O)O

Cette structure est également disponible sous forme de fichier Mol 2d ou sous forme de...

- **D'autres noms:** Isophthalic acid; m-Benzenedicarboxylic acid; m-Phthalic acid; Benzene, 1,3-dicarboxylic acid; Acide isop...
- **Information on this page:**
 - Notes / Error Report
- **Other data available:**
 - Condensed phase thermochemistry data
 - Phase change data
 - Gas phase ion energetics data
 - IR Spectrum
 - Mass spectrum (electron ionization)
 - UV/Visible spectrum
- **Options:**
 - Switch to calorie-based units

Data at NIST subscription sites:

- **NIST / TRC Web Thermo Tables, professional edition** (evaluated thermophysical and...

NIST subscription sites provide data under the **NIST Standard Reference Data Program**, 1 development of data collections included in such sites. Your institution may already be a s...



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

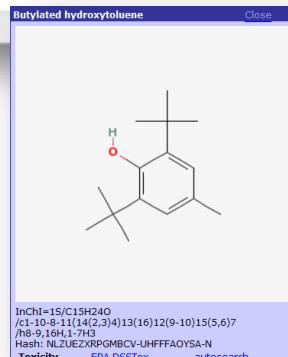
34

PRINCIPLES: 6 MAIN AREAS

Search migrants/data: Migrants (M,SML...) Transport Properties

name/IUPAC

Butylated hydroxytoluene
N,N-Dibutylaniline
Butylated hydroxytoluene



2

Help



Migrant found: Butylated hydroxytoluene

Name: [Butylated hydroxytoluene](#) (Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-;*p*-Cresol, 2,6-di-tert-butyl-;Advastab 401;Antioxidant D...)
CAS: [128-37-0](#)

Formula: C15H24O

M: 220.3505 g/mol

D_P1: 23 values ([view](#))

5

List of available data

23 diffusion coefficient(s) (D_P1 at T1) found.
Legend: P1 = any reference polymer, T1=temperature

| Name | CAS | formula | M | P1 | P2 | value | unit | T1 (°C) | T2 (°C) | rho1 | rho2 | import |
|--------------------------|----------|---------|--------|------|----|-----------|------|---------|---------|-------|------|---------------------------------------|
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 6.600e-14 | m2/s | 23 | | 0.918 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 1.500e-13 | m2/s | 25 | | | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 8.100e-14 | m2/s | 23 | | 0.918 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 3.450e-12 | m2/s | 70 | | 0.918 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 9.000e-14 | m2/s | 25 | | | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 9.600e-14 | m2/s | 23 | | 0.918 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 4.800e-14 | m2/s | 23 | | | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 1.200e-14 | m2/s | 23 | | | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 8.300e-13 | m2/s | 60 | | | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 1.500e-13 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 8.200e-14 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 9.000e-14 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 9.600e-14 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 6.500e-14 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | LDPE | | 6.600e-14 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | MDPE | | 1.000e-10 | m2/s | 40 | | 0.92 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | MDPE | | 1.380e-14 | m2/s | 40 | | 0.94 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | MDPE | | 1.600e-16 | m2/s | 40 | | 0.94 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | MDPE | | 4.800e-16 | m2/s | 40 | | 0.94 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | MDPE | | 5.300e-16 | m2/s | 40 | | 0.94 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | PP | | 4.600e-15 | m2/s | 40 | | 0.95 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | PP | | 2.700e-16 | m2/s | 40 | | 0.95 | | <input type="button" value="import"/> |
| Butylated hydroxytoluene | 128-37-0 | C15H24O | 220.35 | PP | | 5.000e-15 | m2/s | 40 | | 0.95 | | <input type="button" value="import"/> |

Sort values by any field

| T1 (°C) |
|---------|
| 23 |
| 23 |
| 23 |
| 23 |
| 23 |
| 25 |
| 25 |
| 40 |
| 40 |

import

Layer 2

| | | | |
|-----------------|---------|--|---------------------------------------|
| I_P | 5 | μm | <input type="button" value="import"/> |
| rho_P | 1 | kg·m ⁻³ or g·cm ⁻³ | <input type="button" value="import"/> |
| k _{TP} | 1 | <input type="button" value="import"/> | |
| D_P | 1.2e-14 | m ² s ⁻¹ | <input type="button" value="import"/> |
| Conc. | 1000 | ppm | <input type="button" value="import"/> |

Database of diffusion coefficients and partition coefficients for polyolefins (>1300 data)

Sort column contents by clicking on column headers. Values are imported in the active layer.

4



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

35

PRINCIPLES: 6 MAIN AREAS

Search migrants/data: Migrants (M,SML...) Transport Properties

name/IUPAC

Tetradecane
1-Tetradecanol
Tetradecaneamide
Tetradecane
1-Tetradecanol
Isopropyl Myristate
Tetradecanoic acid, methyl est
Tetradecane
Tetradecanoic acid, methyl est

List of available data

Migrant found: Tetradecane

Name: [Tetradecane \(n-Tetradecane...\)](#)
 CAS: [629-59-4](#)
 Formula: C14H30
 M: 198.388 g/mol

D_P1: 9 values ([view](#))
 KP1/P2: 12 values ([view](#))

9 diffusion coefficient(s) (D_P1 at T1) found.
 Legend: P1= any reference polymer, T1=temperature

| Name | CAS | formula | M | P1 | P2 | value | unit | T1 (°C) | T2 (°C) | rho1 | rho2 | import |
|-------------|----------|---------|--------|------|----|------------------|------|---------|---------|-------|------|------------------------|
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | | 1.900e-13 | m2/s | 23 | | 0.918 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | | 2.500e-13 | m2/s | 40 | | 0.92 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | | 1.800e-13 | m2/s | 40 | | 0.92 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | | 1.920e-13 | m2/s | 40 | | 0.92 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | MDPE | | 4.900e-14 | m2/s | 40 | | 0.94 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | MDPE | | 3.100e-14 | m2/s | 40 | | 0.94 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | PP | | 9.200e-15 | m2/s | 40 | | 0.95 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | PP | | 9.200e-15 | m2/s | 40 | | 0.95 | | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | PP | | 9.200e-15 | m2/s | 40 | | 0.95 | | import |

12 partition coefficient(s) (K_P1/P2 at T1) found.
 Legend: P1= one phase (polymer or food simulant), P2= another phase (polymer or food simulant), T1=temperature

| Name | CAS | formula | M | P1 | P2 | value | unit | T1 (°C) | T2 (°C) | rho1 | rho2 | import |
|-------------|----------|---------|--------|------|----------|---------------|-------------|---------|---------|------|------|------------------------|
| Tetradecane | 629-59-4 | C14H30 | 198.39 | HDPE | Ethanol | 21.8 | (m/v)/(m/v) | 10 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | HDPE | Ethanol | 6.17 | (m/v)/(m/v) | 25 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | HDPE | Ethanol | 4.13 | (m/v)/(m/v) | 40 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Ethanol | 9.41 | (m/v)/(m/v) | 10 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Ethanol | 3.47 | (m/v)/(m/v) | 25 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Ethanol | 3.24 | (m/v)/(m/v) | 40 | | 0.96 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Ethanol | 1.30 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Ethanol | 0.0160 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Methanol | 0.0640 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Methanol | 0.0140 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Methanol | 0.0600 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |
| Tetradecane | 629-59-4 | C14H30 | 198.39 | LDPE | Methanol | 0.0660 | (m/v)/(m/v) | 23 | | 0.92 | 0.79 | import |

Sort column content

5



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

36

PRINCIPLES: 6 MAIN AREAS

3

Contact conditions

L_FP 50 kgF·kgP⁻¹ import

V_F 300 cm³ import

A_F 200 cm² import

rho_F 1 kg·m⁻³ or g·cm⁻³ import

k_F 1 import

Bi 1000000 import

t 10 days import

Temperature : set import

3

Contact conditions

L_FP 50 kgF·kgP⁻¹ import

V_F import

A_F import

rho_F 1 kg·m⁻³ or g·cm⁻³ import

k_F 1 import

Bi 1000000 import

t 10 days import

Temperature : set import

5

VF

[SI unit m³]

Volume of F in contact with P

No safe value

AF

[SI unit m²]

Surface of F in contact with P

No safe value

Layer selector

<< < > >> 1

Layer 1

I_P 300 μm import

rho_P 1 kg·m⁻³ or g·cm⁻³ import

K_F/P 1 import T

D_P 1e-014 m²·s⁻¹ import T

Conc. 1000 ppm import

4

GEOMETRICAL FACTORS ARE EITHER
CALCULATED OR IMPLEMENTED AS A
DILUTION FACTOR

L_FP

[SI unit: m³/m³]

Overall volume dilution factor, ratio between the volume of F and the volume of P in contact.

No safe value



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE INPUT FORM

37

PRINCIPLES: 6 MAIN AREAS

Layer selector

<<

<

>

>>

3

NUMBER OF LAYERS
(UP TO 10)

Layer 1

| | | | |
|-------|--------|--|--------|
| I_P | 300 | μm | import |
| rho_P | 1 | kg·m ⁻³ or g·cm ⁻³ | import |
| K_F/P | 1 | import | T |
| D_P | 1e-014 | m ² .s ⁻¹ | import |
| Conc. | 1000 | ppm | import |

4

Layer 2

| | | | |
|-------|----------|--|--------|
| I_P | 0 | μm | import |
| rho_P | 1 | kg·m ⁻³ or g·cm ⁻³ | import |
| K_F/P | 1 | import | T |
| D_P | 8.99e-14 | m ² .s ⁻¹ | import |
| Conc. | 0 | ppm | import |

4

D_P
[SI unit: m²/s]

diffusion coefficient in P

Use the form below as safe value (for the highest temperature).

Piringer Calculator

| | | |
|--|------------|---------------------|
| Polymer: | LDPE | °C |
| T: | 40 | g.mol ⁻¹ |
| M: | 646.921581 | |
| M of tri(2,4-ditert-butylphenoxy)phosphane: 646.921581 | | |
| <input type="button" value="Import in current layer"/> | | |

VALUES CAN BE TYPED, IMPORTED OR CALCULATED

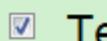


DIFFUSION_1DFV2N.SFPP3.HTML

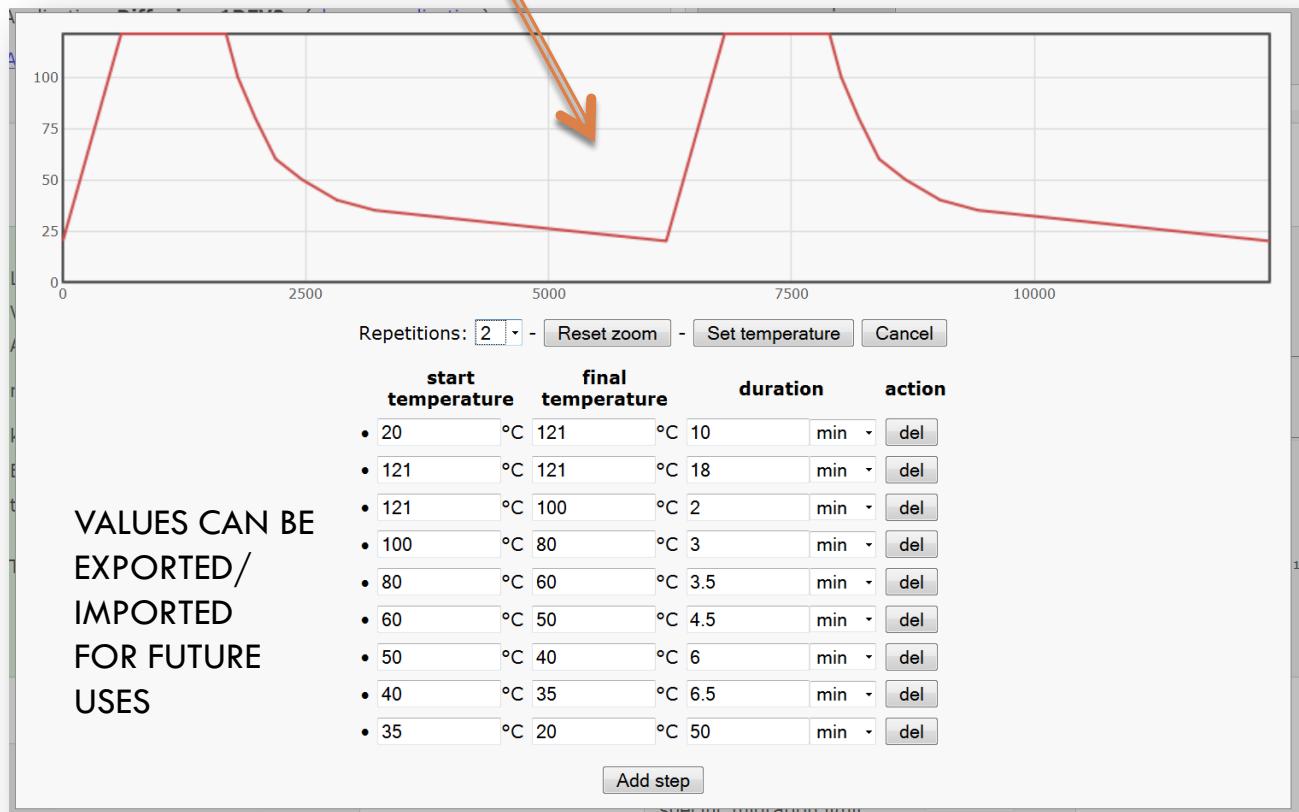
INTERACTIVE INPUT FORM

38

NON ISOTHERM MIGRATION



Temperature :

set**import****3**

VALUES CAN BE
EXPORTED/
IMPORTED
FOR FUTURE
USES

K_F/P **0.1****4****import****T**D_P **1e16****m².s⁻¹****import****T**

ACTIVATION ENERGIES
DEFINITION (HERE FOR D
AROUND A Tg AT 96°C)

Set temperature Cancel

| | Temperature | kJ/mol | action |
|---|-------------|--------|--------|
| • | 0 °C | 85 | del |
| • | 96 °C | 200 | del |
| • | 110 °C | 85 | del |

Add row



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE PLOTS

39

RESULTS PRESENTATION

My Information

My user : demouser ([change user](#))
 My project : Diffusion_1DFV2n ([change project](#))
 My database : common.sfpp3.database
 My Application : common ([change application](#))

INRA\SFPP3 - 16-May-2009 17:34:24

Current simulation result

diffusion_1DFFn_16-May-2009_17-34-24_6610

[Rename](#) [Delete](#)

>>> EXCEL™ file <<<

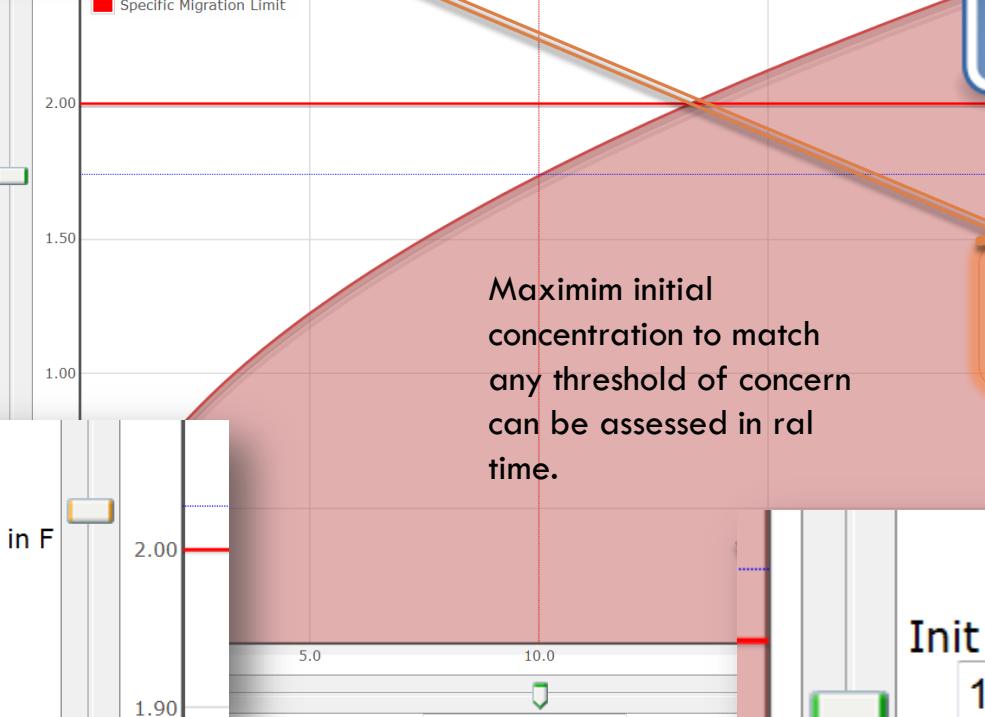
>>> PDF document <<<

[New simulation](#)

1

2

[Image results](#)
[Simulation report](#)
[kinetic graph](#)
[profile graph](#)
[Reset zoom](#)
 Show cursors
 Resolution: high average low[Reset zoom](#)
 Show cursors

 Concentration in F
 2.44
 1.74
 0 ppm

 Concentration in F
 2.27
 2.03
 1.68 ppm

 Init Conc in P
 1.60e+3
 reset
 ppm

Init Conc in P

1.87e+3

[reset](#)

ppm

Time : 8.19 - 9.75 - 11 days



DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE PLOTS

40

RESULTS PRESENTATION

My Information

My user : demouser ([change user](#))
 My project : Diffusion_1DFV2n ([change project](#))
 My database : common.sfpp3.database
 My Application : common ([change application](#))

INRA\SFPP3 - 16-May-2009 17:34:24

Current simulation result

diffusion_1DFFn_16-May-2009_17-34-24_6610

[Rename](#) [Delete](#)

>>> EXCEL™ file <<< >>> PDF document <<<

[New simulation](#)

2

Image results

Simulation report

kinetic graph

profile graph

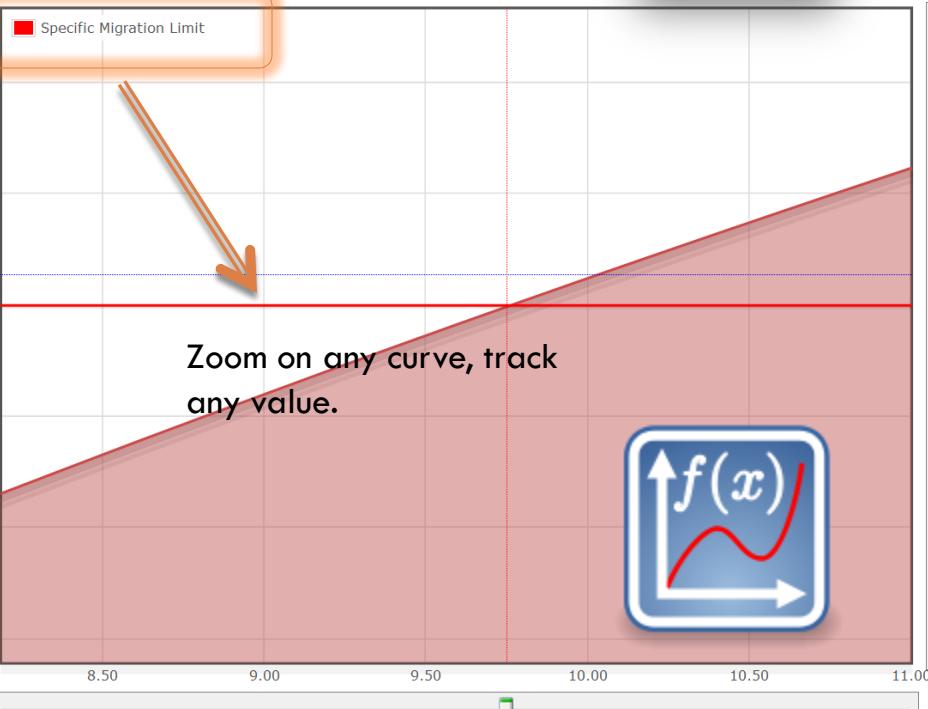
Change quality of plots: high = 10^4 points

Resolution: high average low

Resolution: high average low[Reset zoom](#) - Show cursors[Reset zoom](#)

Concentration in F
2.27
2.03
1.68
ppm

Init Conc in P
1.87e+3
[reset](#)
ppm





DIFFUSION_1DFV2N.SFPP3.HTML

INTERACTIVE PLOTS

41

RESULTS PRESENTATION

My Information

My user : demouser ([change user](#))
 My project : Diffusion_1DFV2n ([change project](#))
 My database : common.sfpp3.database
 My Application : common ([change application](#))

INRA\SFPP3 - 16-May-2009 17:34:24

Current simulation result

diffusion_1DFFn_16-May-2009_17-34-24_6610

[Rename](#) [Delete](#)

>>> EXCEL™ file <<<

>>> PDF document <<<

[New simulation](#)

2

Image results

Simulation report

kinetic graph

profile graph

Add curves and
change their colors

Test_for_Catherine

Test_for_Catherine100 [delete](#)Test_for_Catherine [delete](#)

Reso





42

SFFP2 APPLICATIONS SUPPORTED IN SFPP3

These applications have been developed for educational purposes and were freely available on internet.

APPLICATIONS

Migration from monolayers

43

Diffusion_1DFV.sfpp3.html

SFPP3 VERSION (WEB VERSION)

It simulates the desorption from **monolayer** materials (denoted P) in food or food simulants (denoted F).

F = liquid, semi-liquid (gel), solid.

Features:

- diffusion control in P
- partitioning between P and F
- mass transfer resistance on food side
- All notations are explained
- Recommended values are proposed
- Calculate kinetics and profiles
- Calculates times required to reach prescribed migration rates
- Results can be exported in **PDF and XLS**
- All input parameters can be saved on client side for a future use.
- Connection to databases requires the web version

- Sort applications by name
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomato
- Other applications



Diffusion_1DFVx.sfpp3.html

SFPP3 VERSION (WEB VERSION)

A simplified interface to the desorption from **monolayer** materials (denoted P) in food or food simulants (denoted F). Initial rough assumptions can be progressively refined according to additional knowledge.

F = liquid, semi-liquid (gel), solid.

Features:

- add partitioning effect
- add diffusion-controlled effect
- add food texture effect
- All notations are explained
- Recommended values are proposed
- Calculates kinetics and profiles
- Calculates times required to reach prescribed migration rates
- Results can be exported in **PDF and XLS**
- Connection to databases requires the web version



APPLICATIONS

Migration from multilayers

44

[Diffusion_1DFVn.sfpp3.html](#)

SFPP3 VERSION (WEB VERSION)

- Sort applications by name
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- **Diffusion_1DFVn.sfpp3.html**
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

It simulates the desorption from **multilayer** materials (denoted P) in food or food simulants (denoted F).

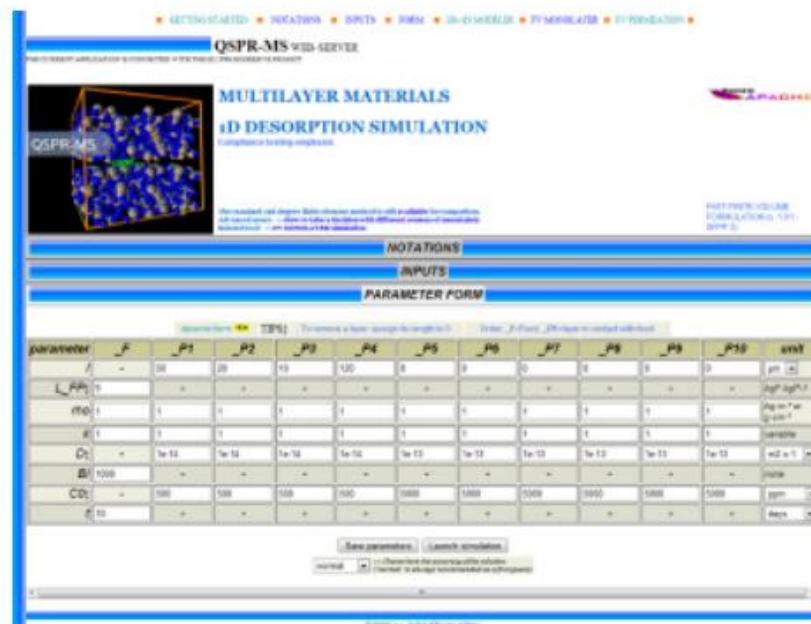
P = multilayer and/or multimaterials consisting in up to 10 layers

F = liquid, semi-liquid (gel), solid.

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- physical formulation is based on Henry's law instead of arbitrary partition coefficients
- mass conservative numerical scheme
- very fast code
- the numerical accuracy can be controlled by the user
- All notations are explained
- Recommended values are proposed
- Calculates kinetics and profiles
- Theoretical equilibrium values are calculated
- Results can be exported in **PDF** and **XLS**
- All input parameters can be saved on client side for a future use.
- Connection to databases requires the web version



APPLICATIONS

Migration from multilayers

45

- Sort applications by name

- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

[Diffusion_1DFVnx.sfpp3.html](#)

SFPP3 VERSION (WEB VERSION)

An interactive interface to the desorption from **multilayer** materials (denoted P) in food or food simulants (denoted F).

The user can add dynamically up to 10 layers.

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- ideal for simple bilayer and trilayer materials
- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- physical formulation is based on Henry's law instead of arbitrary partition coefficients
- mass conservative numerical scheme
- very fast code
- the numerical accuracy can be controlled by the user
- All notations are explained
- Recommended values are proposed
- Calculates kinetics and profiles
- Theoretical equilibrium values are calculated
- Results can be exported in **PDF** and **XLS**
- Connection to databases requires the web version

The screenshot shows a web-based application for "MULTILAYER MATERIALS 1D DESORPTION SIMULATION". The interface includes a navigation bar with links like "GETTING STARTED", "NOTATIONS", "INPUTS", "PARAMETER FORM", "RESULTS", "DOCUMENTATION", "PUBLICATIONS", and "PURIFICATION". Below the navigation is a section titled "NOTATIONS" with a diagram of a stack of layers labeled "QSPR-MS" and "Food". The "PARAMETER FORM" section contains a table with parameters: J (µm/s), λ_{PF} (kg m⁻² s⁻¹), ρ_{FOOD} (kg m⁻³), R (variable), D_F (m² s⁻¹), D_B (none), C_0 (ppm), and t (days). Buttons for "Save parameters", "Launch simulation", and "Results" are visible at the bottom.

APPLICATIONS

3D MODELING FOR SIMULATION

46

- Sort applications by name

- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

[food3D.sfpp3.html](#)

SFPP3 VERSION (WEB VERSION)

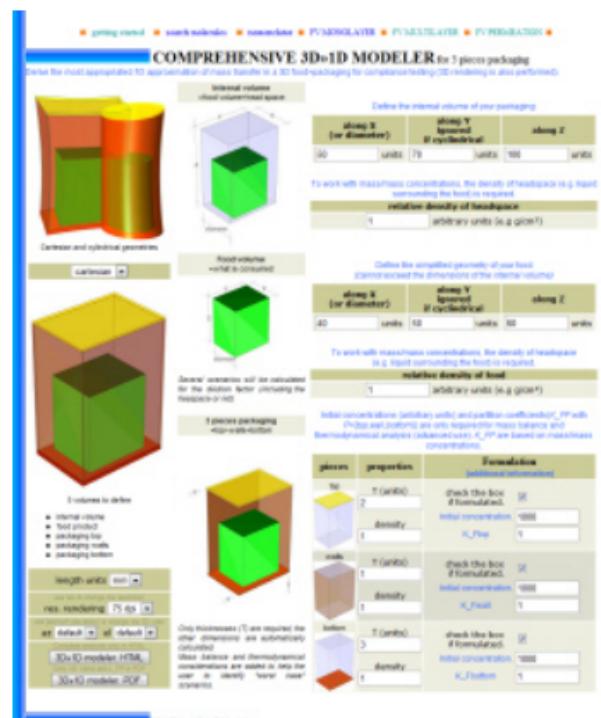
All migration simulation tools describe 1D transport whereas they are 3D in a complex food packaging. This tool calculates the best 1D approximation for a 3 pieces packaging (including a top, walls and a bottom) while taking into account the geometry of the food and of the headspace.

The geometry is fully rendered in 3D with transparencies with arbitrary camera position (if you video card handle opengl).

The approximations are calculated for three assumptions: i) the migration is involved in whole inner volume, ii) in the head space only, iii) in the food only.

Features:

- the geometries of the food product and of the head space are considered
- each piece of the packaging can consist in a different material with different properties and formulation
- cartesian and cylindrical coordinates are considered
- dilution factor and concentration values at thermodynamical equilibrium are calculated for any configuration
- All notations are explained
- 3D views with transparencies and legends
- rendering at customizable resolution and camera position
- Numerical data and 3D views can be generated in PDF to be included in a report.



APPLICATIONS PERMEATION

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[Permeation_1DFVn.sfpp3.html](#)

- Sort applications by name
- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- **Permeation_1DFVn.sfpp3.html**
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

SFPP3 VERSION (WEB VERSION)

Simulates the sorption, diffusion and desorption process (so-called **permeation**) between two compartments (finite or infinite), denoted FA and FB. The traversed medium, denoted P, may include up to 10 different layers (**multilayer materials**).

P = multilayer and/or multimaterials consisting in up to 10 layers
 FA, FB= liquid, semi-liquid (gel), solid.

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- possible external mass transfer resistances are considered
- finite volume effects are considered
- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- mass conservative numerical scheme
- very fast code
- the numerical accuracy can be controlled by the user
- All notations are explained
- Calculates kinetics in FA and in FB and profiles in P
- Results can be exported in **PDF** and **XLS**
- All input parameters can be saved on client side for a future use.
- Connection to databases requires the web version



The screenshot shows the QSPR-MS Web-Server interface. At the top, there's a navigation bar with links: READING-HEARTED, INPUT, FORM, 1D-DF-NODELER, SORPTION/DESORPTION SIMULATOR, and DESORPTION/DF-MULTILAYER. Below the navigation bar, there's a banner for MULTILAYER MATERIALS, followed by three buttons: 1D PERMEATION SIMULATION, 1D SORPTION/DESORPTION SIMULATION, and 1D DIFFUSION SIMULATION. The main area is titled "INPUTS" and contains a "PARAMETER FORM" table. The table has columns for parameters and values, with some cells containing mathematical expressions like t_{FA} , P_1 , D , C_0 , and t_{FB} . There are also dropdown menus for "TIPS" and "Boundary conditions". At the bottom of the form, there are buttons for "Save parameters" and "Launch simulation". A note at the bottom right says "©2007 by INRA/Olivier Vitrac".

APPLICATIONS PERMEATION

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- Sort applications by name

- Diffusion_1DFV.sfpp3.html
- Diffusion_1DFVx.sfpp3.html
- Diffusion_1DFVn.sfpp3.html
- Diffusion_1DFVnx.sfpp3.html
- food3D.sfpp3.html
- Permeation_1DFVn.sfpp3.html
- Permeation_1DFVnx.sfpp3.html
- Adhesive
- Tomate
- Other applications

[Permeation_1DFVnx.sfpp3.html](#)

SFPP3 VERSION (WEB VERSION)

Interactive interface to **permeation** simulation. Up to 10 layers can be added (**multilayer materials**).

P = multilayer and/or multimaterials consisting in up to 10 layers

FA, FB= liquid, semi-liquid (gel), solid.

The implementation is based on very efficient Finite Volume (FV) solution combining semi-analytical solutions.

Features:

- possible external mass transfer resistances are considered
- finite volume effects are considered
- no limitation in size for each layer (a thin 10 nm thick layer can be combined with a 100 µm layer)
- large discrepancies in transport properties are tolerated
- mass conservative numerical scheme
- very fast code
- the numerical accuracy can be controlled by the user
- All notations are explained
- Calculates kinetics in FA and in FB and profiles in P
- Results can be exported in **PDF and XLS**
- All input parameters can be saved on client side for a future use.
- Connection to databases requires the web version

| parameter | unit/cale | FA | FB | Pg |
|-----------------|--------------------------------|------|------|-------|
| \bar{f} | pm | - | - | 50 |
| L_{FA} | m ² s ⁻¹ | 10 | 10 | - |
| β | kg m ⁻² | 1 | 1 | 1 |
| k or S | m ⁻¹ | 1 | 1 | 1 |
| D or α | m ² s ⁻¹ | x | x | 1e-12 |
| B | none | 1000 | 1000 | - |
| CD or ρ_0 | ppm | 500 | 0 | 0 |
| E | days | 10 | - | - |

Buttons at the bottom include 'Save parameters' and 'Launch simulation'. A note says 'Please choose the simulation of the database "Tomate" to obtain the simulation results in a new window'.

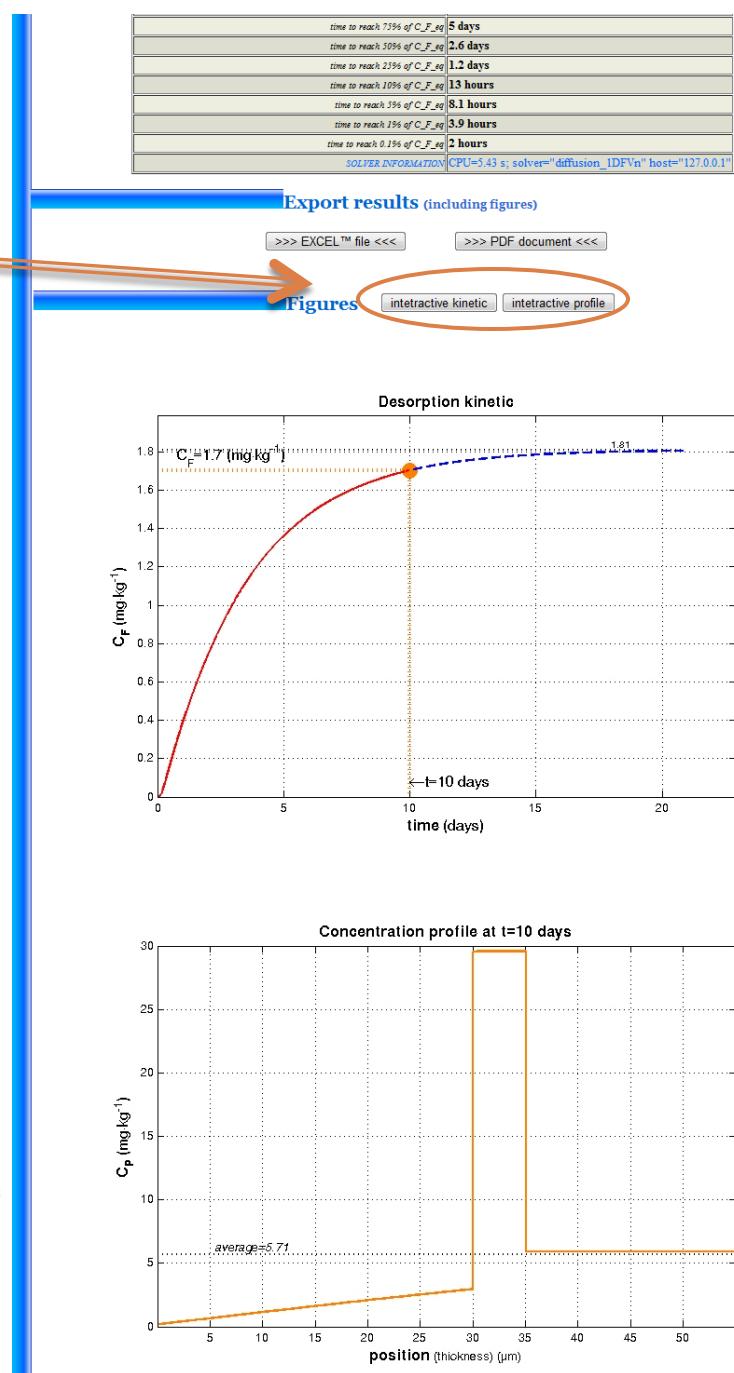
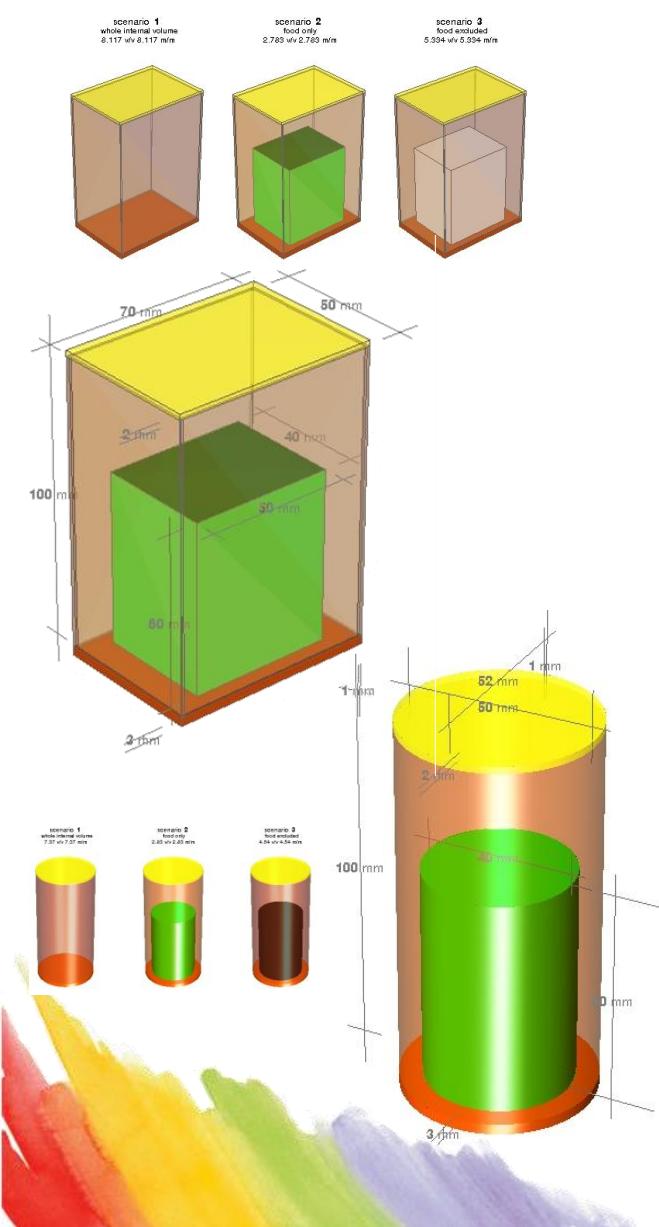
Edited by Olivier Vitrac

2D/3D PLOTS IN SFPP3

IMAGES OR INTERACTIVE VECTORIAL PLOTS

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Along simulations, SFPP3 generates 2D or 3D or plots as static images. Dynamic plots can also be generated a posteriori from any previous results.



2D/3D PLOTS IN SFPP3

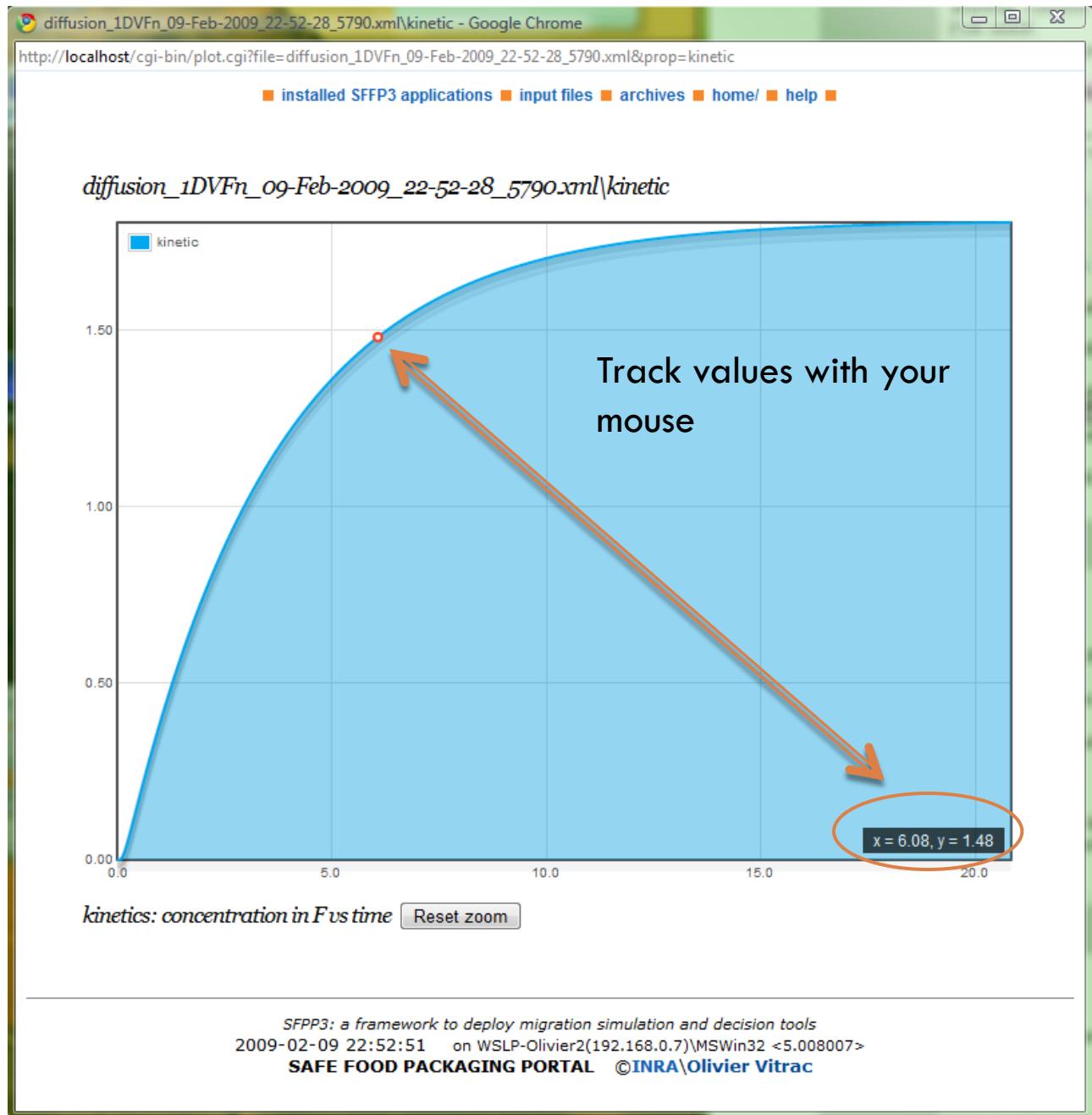
IMAGES OR INTERACTIVE VECTORIAL PLOTS

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Figures

intetraactive kinetic

intetraactive profile



2D/3D PLOTS IN SFPP3

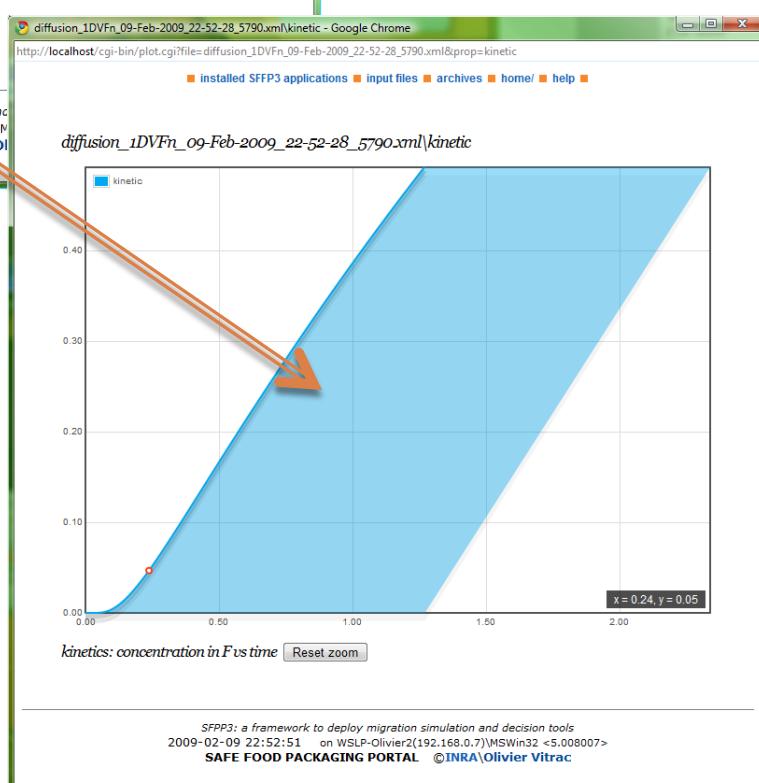
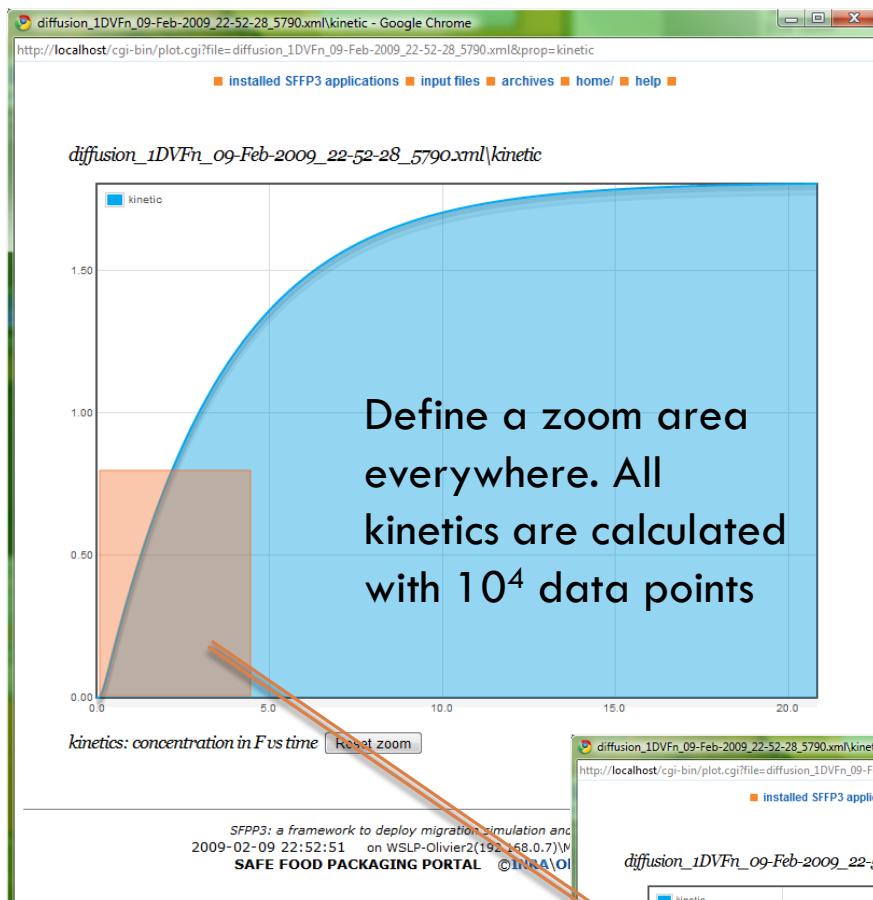
IMAGES OR INTERACTIVE VECTORIAL PLOTS

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Figures

intetraction kinetic

intetraction profile



2D/3D PLOTS IN SFPP3

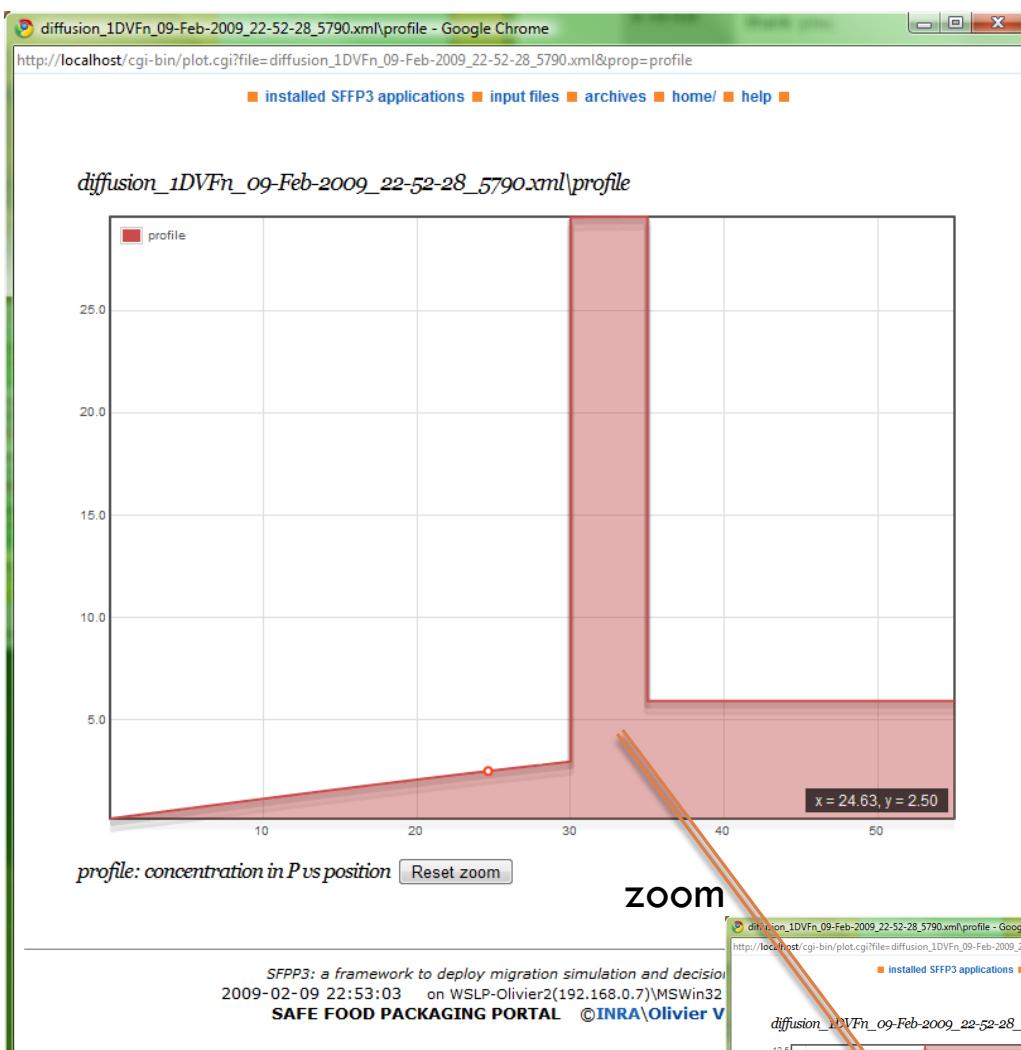
IMAGES OR INTERACTIVE VECTORIAL PLOTS

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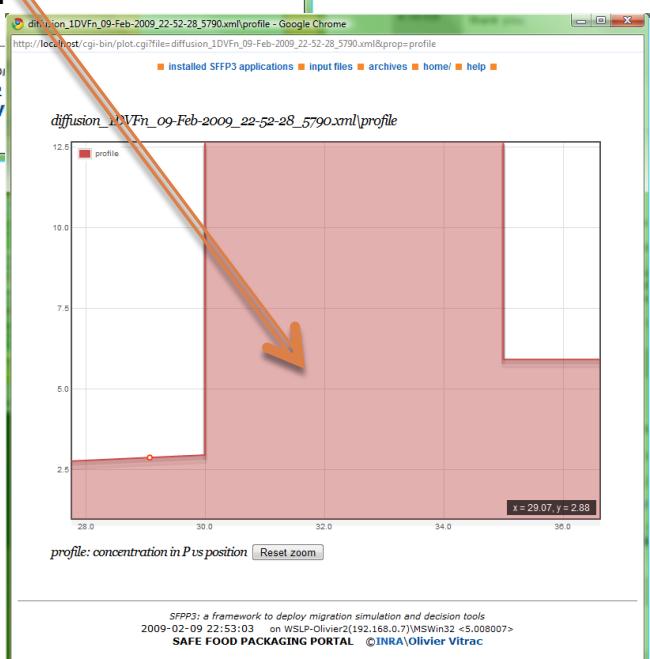
Figures

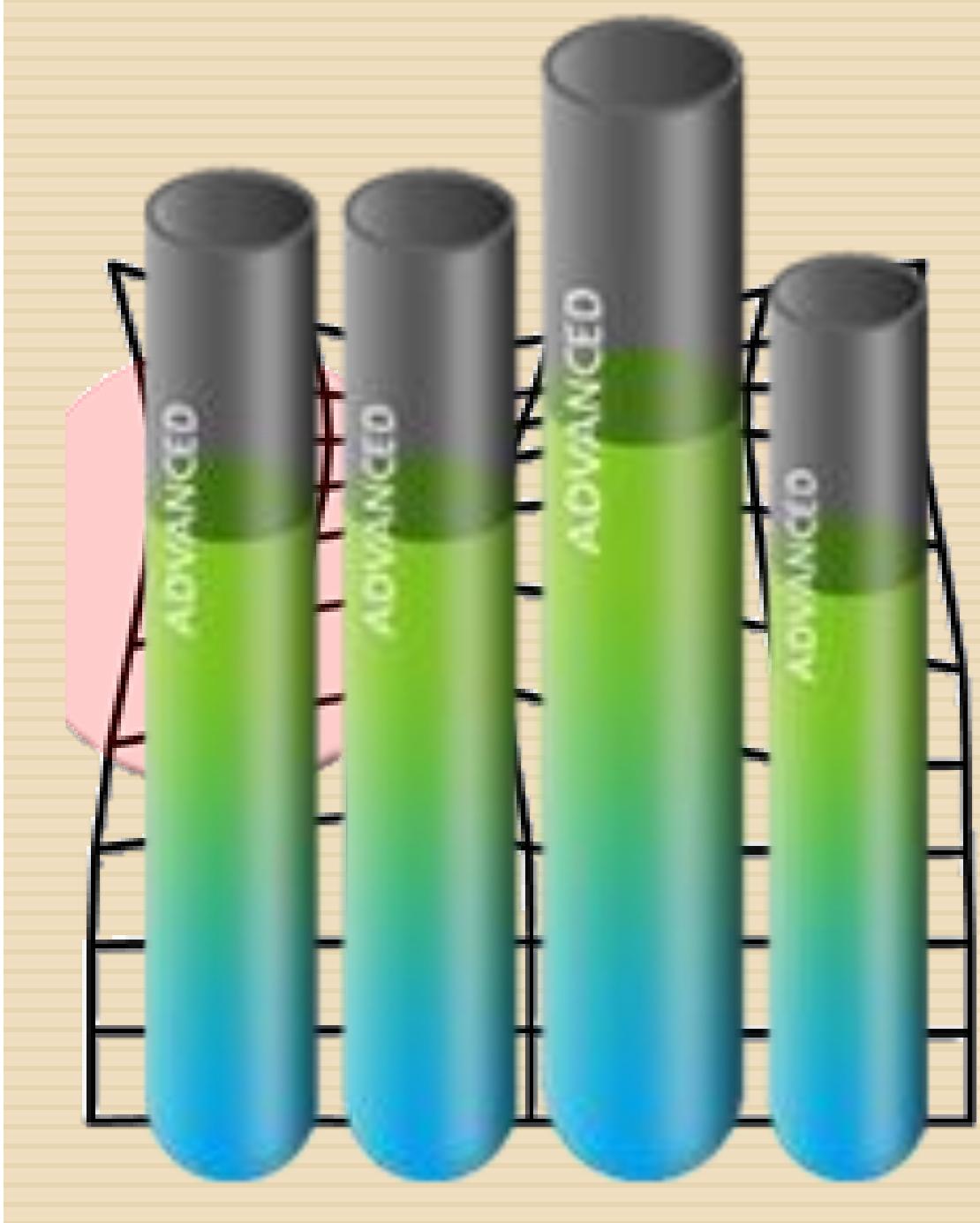
intetraactive kinetic

intetraactive profile



Concentration profiles
include between 50
and 300 data points.





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ADVANCED USER INTERFACE

MANAGING JOB AND ARCHIVE FILES

TRACEABILITY OF DATA

REPORTING

Main menu: <http://localhost>

List all installed SFPP3 applications

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DEFAULT MENU based on index.cgi



SFPP.cgi



my input file



myresult.xml



home

- [installed SFPP3 applications](#)
- [input files](#)
- [archives](#)
- [home/](#)
- [map](#)
- [help](#)
- [debug](#)
- [»Logout«](#)

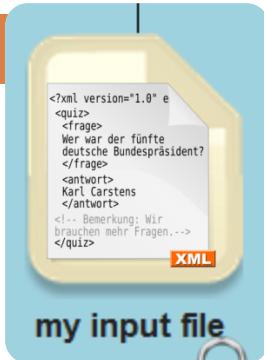
home/*.SFPP3.html

project=[*Common*](#)
(database=[*common.sfpp3.database.xml*](#)*)*

| Application or Object | Date | Size (bytes) |
|---|--------------------------|--------------|
| Diffusion_1DFV.sfpp3 | Tue Jan 20 14:20:24 2009 | 22211 |
| Diffusion_1DFVn.sfpp3 | Tue Jan 20 14:20:34 2009 | 40660 |
| Diffusion_1DFVnx.sfpp3 | Tue Jan 20 14:20:54 2009 | 25226 |
| Diffusion_1DFVx.sfpp3 | Tue Jan 20 14:21:04 2009 | 22402 |
| Diffusion_out.sfpp3 | Sun Jan 18 19:11:44 2009 | 5614 |
| food3D.sfpp3 | Mon Jan 19 22:59:01 2009 | 14313 |
| permeation_1DFVn.sfpp3 | Sun Jan 18 17:20:37 2009 | 32308 |
| permeation_1DFVnx.sfpp3 | Sun Jan 18 18:09:54 2009 | 17624 |
| Piringer.sfpp3 | Sun Jan 18 15:02:57 2009 | 5683 |

List all previous jobs

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Click on job a name to get a detailed view.

- [installed SFPP3 applications](#)
- [input files](#)
- [archives](#)
- [home/](#)
- [help](#)
- [debug](#)
-

cgi-bin/infile/*.xml

(refresh this page if required)

| Application or Object | Date | Size (bytes) | action | action | action |
|--|--------------------------|--------------|---------------------|---------------------|------------------------|
| SFPP_2009-01-24_23-30-53-3522.infile | Sun Jan 25 00:38:06 2009 | 1299 | xml | run | delete |
| SFPP_2009-01-24_23-39-03-2552.infile | Sun Jan 25 00:39:03 2009 | 1299 | xml | run | delete |
| SFPP_2009-01-25_16-53-10-8749.infile | Sun Jan 25 17:53:10 2009 | 1631 | xml | run | delete |
| SFPP_2009-01-25_16-54-48-7774.infile | Sun Jan 25 17:54:48 2009 | 1243 | xml | run | delete |
| SFPP_2009-01-25_19-42-46-9495.infile | Sun Jan 25 20:42:46 2009 | 2656 | xml | run | delete |
| SFPP_2009-01-25_19-43-25-8588.infile | Sun Jan 25 20:43:25 2009 | 2877 | xml | run | delete |
| SFPP_2009-01-25_19-53-35-4008.infile | Sun Jan 25 20:53:35 2009 | 2145 | xml | run | delete |
| SFPP_2009-01-25_20-52-27-5908.infile | Sun Jan 25 21:52:27 2009 | 1751 | xml | run | delete |
| SFPP_2009-01-26_11-54-32-7015.infile | Mon Jan 26 12:54:32 2009 | 2822 | xml | run | delete |
| SFPP_2009-01-26_11-55-40-5920.infile | Mon Jan 26 12:55:40 2009 | 1543 | xml | run | delete |
| SFPP_2009-01-26_11-56-21-5360.infile | Mon Jan 26 12:56:21 2009 | 3051 | xml | run | delete |
| SFPP_2009-01-26_11-57-00-5930.infile | Mon Jan 26 12:57:00 2009 | 1543 | xml | run | delete |
| SFPP_2009-01-26_16-37-30-2287.infile | Mon Jan 26 17:37:30 2009 | 2138 | xml | run | delete |
| SFPP_2009-01-26_16-38-16-8579.infile | Mon Jan 26 17:38:16 2009 | 1543 | xml | run | delete |
| SFPP_2009-01-27_15-50-19-7456.infile | Tue Jan 27 16:50:19 2009 | 1324 | xml | run | delete |
| SFPP_2009-01-27_15-59-09-6613.infile | Tue Jan 27 16:59:09 2009 | 1023 | xml | run | delete |
| SFPP_2009-01-27_15-59-52-3348.infile | Tue Jan 27 16:59:52 2009 | 1022 | xml | run | delete |
| SFPP_2009-01-27_16-00-27-3161.infile | Tue Jan 27 17:00:27 2009 | 1023 | xml | run | delete |
| SFPP_2009-01-27_16-09-40-5532.infile | Tue Jan 27 17:09:40 2009 | 1023 | xml | run | delete |
| SFPP_2009-01-27_16-11-07-2862.infile | Tue Jan 27 17:11:07 2009 | 926 | xml | run | delete |
| SFPP_2009-01-29_17-11-09-3780.infile | Thu Jan 29 18:11:09 2009 | 2977 | xml | run | delete |

EXAMPLE OF INPUT FILE

App: DIFFUSION_1DFVnx.sfpp3

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Detailed view with options

■ [installed SFPP3 applications](#) ■ [input files](#) ■ [archives](#) ■ [home/](#) ■ [help](#)

INPUT FILE

[SFPP_2009-01-25_20-52-27-5908.infile.xml](#)

include hidden fields (undefined keys are removed)

| KEYWORD | VALUE |
|--------------|---|
| Bi | 1000 |
| CGI | Q:/SFPP3/html/www/cgi-bin/SFPP.cgi |
| CONTENT | application/x-www-form-urlencoded |
| COOKIE | mvalue/home/Diffusion_1DFV_sfpp3.html=200 9 1 1e-14 1000 500 10 100; mvalue/home/Diffusion_1DFVnx.sfpp3.html=50 20 9 1 1 14 1000 500 10 100 |
| C_P01 | 500 |
| C_P02 | 500 |
| C_P03 | 500 |
| C_P0_unit | ppm |
| DATE | 2009-01-25 21:52:27 |
| DOCUMENTROOT | |
| D_P1 | 1e-14 |
| D_P2 | 1e-14 |
| D_P3 | 1e-14 |
| D_P_unit | m2.s-1 |
| HOST | 127.0.0.1 |
| HTTP | 10 |
| L_FP | 9 |
| METHOD | POST |
| MIME | 7 |
| PAGE | http://localhost/home/Diffusion_1DFVnx.sfpp3.html |
| PORT | 80 |
| QUERY | mlmfile=diffusion_1DFVn;l_P_unit=%B5m;l_P1=50;l_P2=1e-14;l_P3=1e-14;Bi=1000;C_P0_unit=p |
| REMOTEADDR | 127.0.0.1 |
| REMOTEHOST | 127.0.0.1 |
| SCRIPT | /cgi-bin/SFPP.cgi |
| SECURITY | SFPP\©INRA/Olivier Vitrac 2009 |
| SERVER | localhost |
| SERVER | Apache/2.0.54 (Win32) mod_perl/2.0.1 Perl/v5.8.7 |
| Submit | Launch simulation |
| k0 | 1 |
| k1 | 1 |
| k2 | 1 |
| k3 | 1 |
| L_P1 | 50 |
| L_P2 | 20 |
| L_P3 | 50 |
| L_P_unit | um |
| mesh | normal |
| mlmfile | diffusion_1DFVn |
| r0 | 1 |
| r1 | 1 |
| r2 | 1 |
| r3 | 1 |
| rootdir | Q:/SFPP3/html/www/ |
| t | 10 |
| t_unit | days |

run this job

delete this job

view as XML

[run this job](#) [delete this job](#) [view as XML](#)

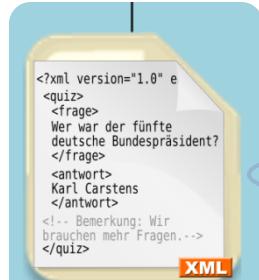
Archives Manager



AJAX compliant (XML-based)

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Tools to manage your simulated results: view, plot, export, delete



called SFPP3 applications ■ input files ■ archives ■ home/ ■ help ■ »Logout« ■

ARCHIVES MANAGER

default: /home/archive/QSPR_arc2009.xml (view, other projects)

REQUEST and PLOT to navigate through simulation details. Raw XML files are best viewed in IE7 or FF3.
Convert in one click your simulation results in PDF or XLS.

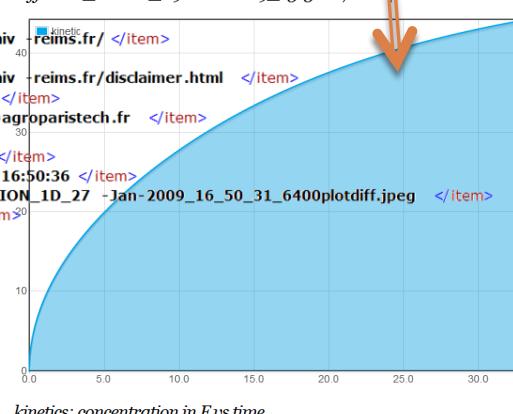
| id | name | tags | summary | kinetics | profile | inputs | PDF | XLS | action |
|----|--------------------------------------|-------------------|---|----------|---------|--------|-----|-----|--------|
| 1 | myresult.xml | Jan-2009_12-54-46 | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 2 | diffusion_1DVFn_26-Jan-2009_12-56-28 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 3 | diffusion_1DVFn_26-Jan-2009_17-37-45 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 4 | diffusion_1D_27-Jan-2009_16-50-36 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 5 | diffusion_1D_29-Jan-2009_15-14-07 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 6 | diffusion_1DVFn_29-Jan-2009_15-32-07 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 14 | diffusion_1D_03-Feb-2009_11-09-06 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 15 | diffusion_1DVFn_03-Feb-2009_11-10-06 | | request view request view plot request view plot request view request view export convert | | | | | | delete |
| 16 | diffusion_1DVFn_03-Feb-2009_11-14-15 | | request view request view plot request view plot request view request view export convert | | | | | | delete |

SFPP3, a framework to deploy migration simulation and decision tools
2009-02-05 10:26:24 testuser on WSLP-Olivier2(10.18.3.100)\MSWin32 <5.008007>
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac

```
<?xml version="1.0" ?>
<!-- SFPP3\INRA-Olivier Vitrac 2009-01-27 18:47:10 -->
<opt idx="10 2" type ="cell">
<item idx="1" size="1 21" type ="char">>Safe Packaging Portal </item>
<item idx="2" size="1 20" type ="char">>Results are provided </item>
<item idx="3" size="1 10" type ="char">>disclaimer </item>
<item idx="4" size="1 7" type ="char">>contact </item>
<item idx="5" size="1 6" type ="char">>e-mail </item>
<item idx="6" size="1 6" type ="char">>----- </item>
<item idx="7" size="1 6" type ="char">>caller </item>
<item idx="8" size="1 4" type ="char">>date </item>
<item idx="9" size="1 4" type ="char">>link </item>
<item idx="10" size="1 4" type ="char">>host </item>
<item idx="11" size="1 25" type ="char">>http://h29.univ-reims.fr/ </item>
<item idx="12" size="1 5" type ="char">>AS IS </item>
<item idx="13" size="1 40" type ="char">>http://h29.univ-reims.fr/disclaimer.html </item>
<item idx="14" size="1 14" type ="char">>Olivier Vitrac </item>
<item idx="15" size="1 31" type ="char">>olivier.vitrac@agroparistech.fr </item>
<item idx="16" size="1 6" type ="char">>----- </item>
<item idx="17" size="1 12" type ="char">>diffusion_1D </item>
<item idx="18" size="1 20" type ="char">>27-Jan-2009 16:50:36 </item>
<item idx="19" size="1 56" type ="char">>/tmp/DIFUSION_1D_27-Jan-2009_16_50_31_6400plotdiff.jpeg </item>
<item idx="20" size="1 9" type ="char">>127.0.0.1 </item>
```



diffusion_1DVFn_29-Jan-2009_15-32-07.xml kinetics





INTERACTIVE PLOTTING

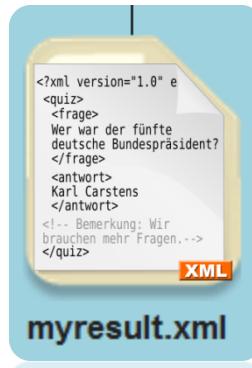


JavaScript framework

Using Prototype Javascript Framework

INTERACTIVE PLOTS IN THE CLIENT BROWSER

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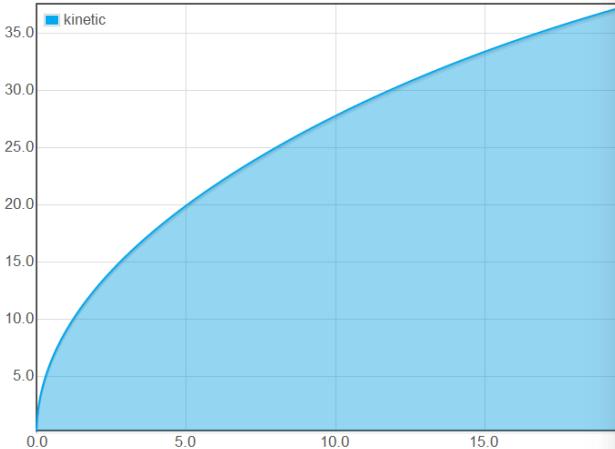


myresult.xml

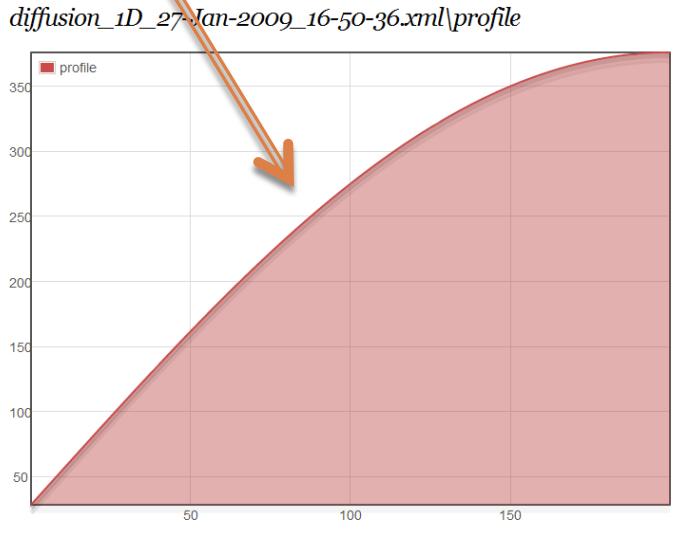
max.js

installed SFFP3 applications input files archives home/ help

diffusion_1D_27-Jan-2009_16-50-36.xml|kinetics



kinetics: concentration in F vs time



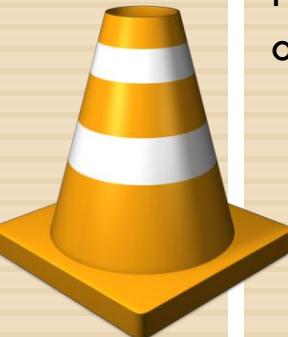
SFPP3: a framework to deploy migration simulation and decision tools
2009-02-01 10:33:28 on WSLP-Olivier2(192.168.0.16)\MSWin32 <5.000807>
SAFE FOOD PACKAGING PORTAL ©INRA Olivier Vitrac



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DEVELOPER MANUAL

Here you will find how to configure SFPP3 and to add your own applications, to create online tutorials...





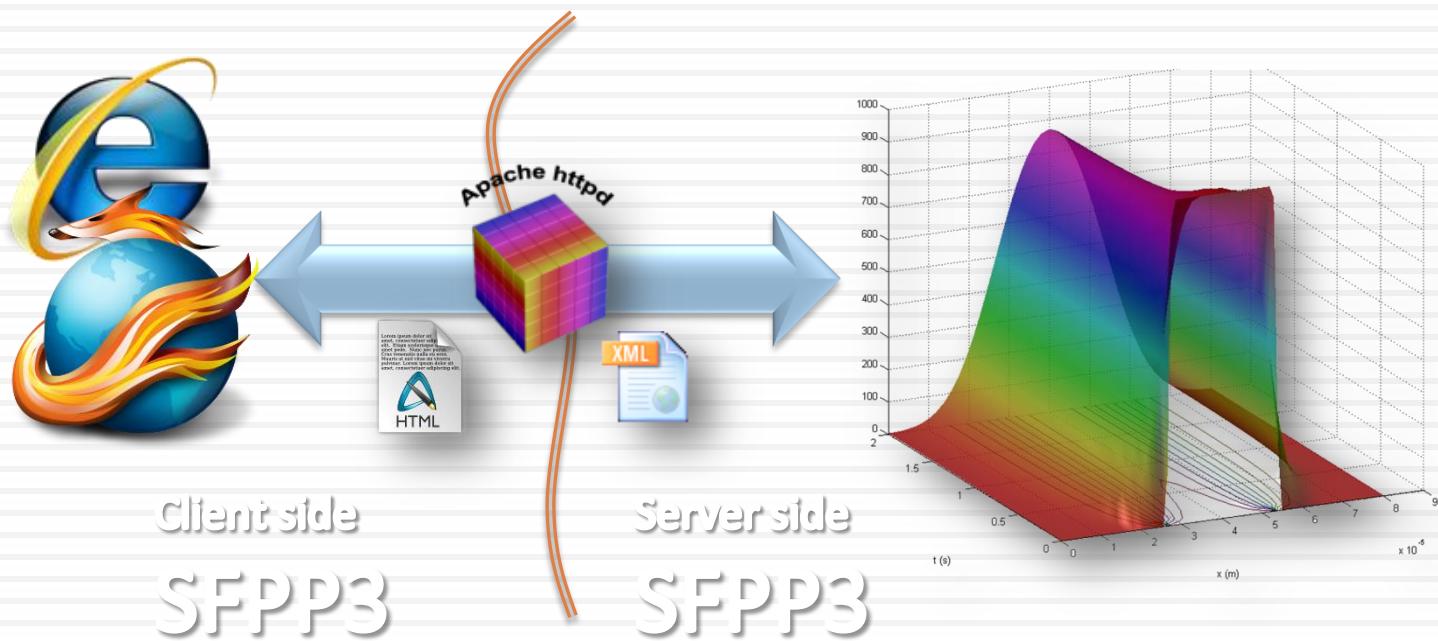
Author: Olivier Vitrac, PhD
Chargé de Recherche INRA

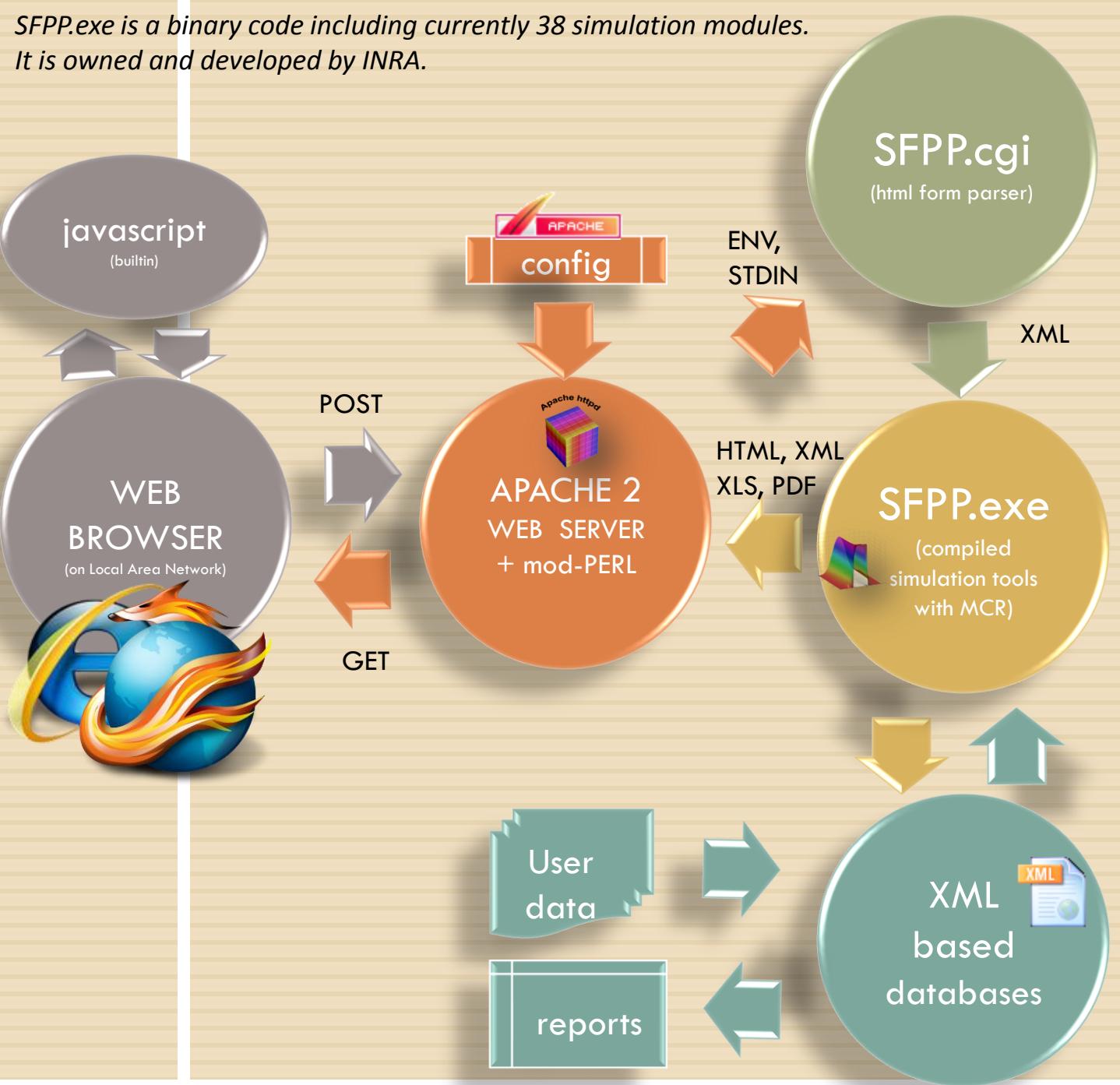
INRA, UMR 1145
Food Process Engineering Joint Research Unit
Agroparistech, site de Massy
1, avenue des Olympiades
91744 Massy cedex, France

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CONTENT FOR DEVELOPERS

- ❖ ARCHITECTURE, SETUP
- ❖ OLD/NEW SFPP3 APPLICATION MODEL
- ❖ DATA MODEL AND ONLINE REQUEST BUILDER
- ❖ ONLINE DEBUGGING TOOLS





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WHAT IS SFPP3? WHY SFPP3?

SFPP3 is a framework to demonstrate the complete feasibility of a distributable standalone application based on the web-components already published online on the SAFE FOOD PACKAGING PORTAL version 2 (SFPP2) (<http://h29.univ-reims.fr>).

SFPP3 works on Win 32/64, Linux 32/64 as a standalone or as a server application.

SFPP3 ANATOMY

from installation folders to web pages



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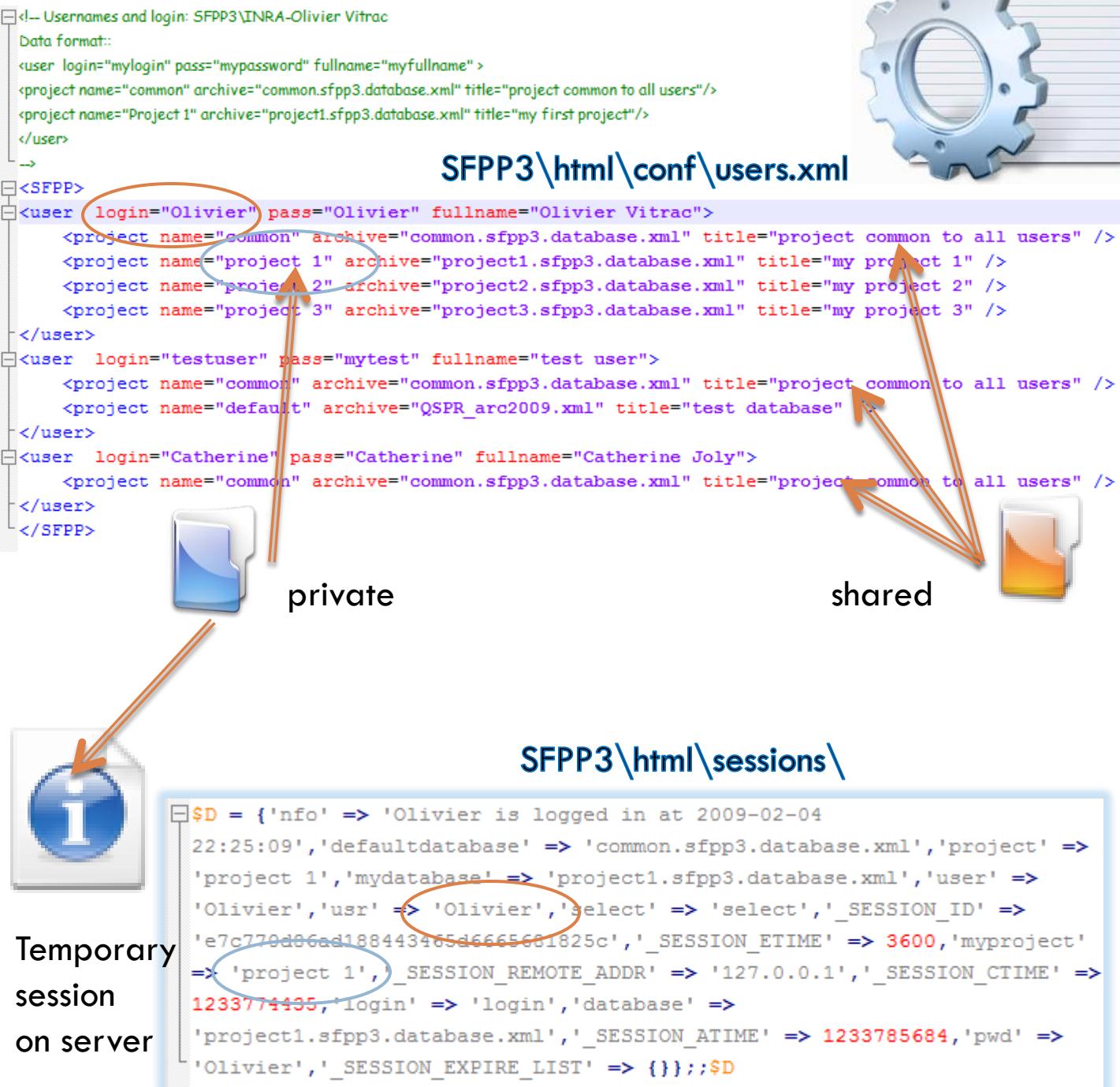


SFPP3: basic setup

user account and project access

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A project = a collection of different simulation results

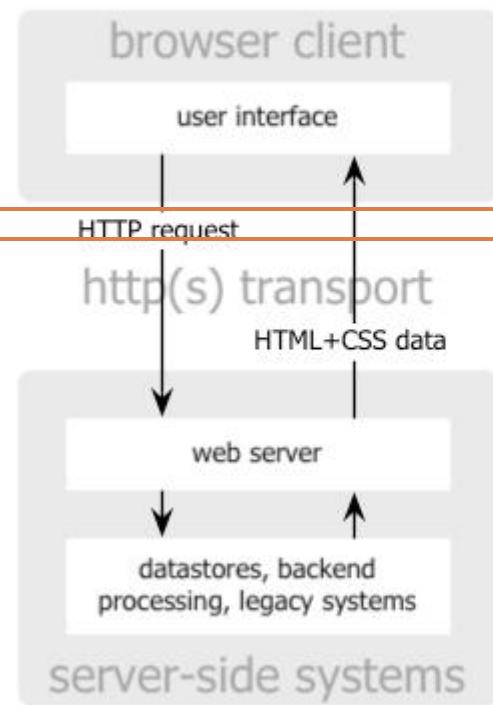


SFPP3: new application model

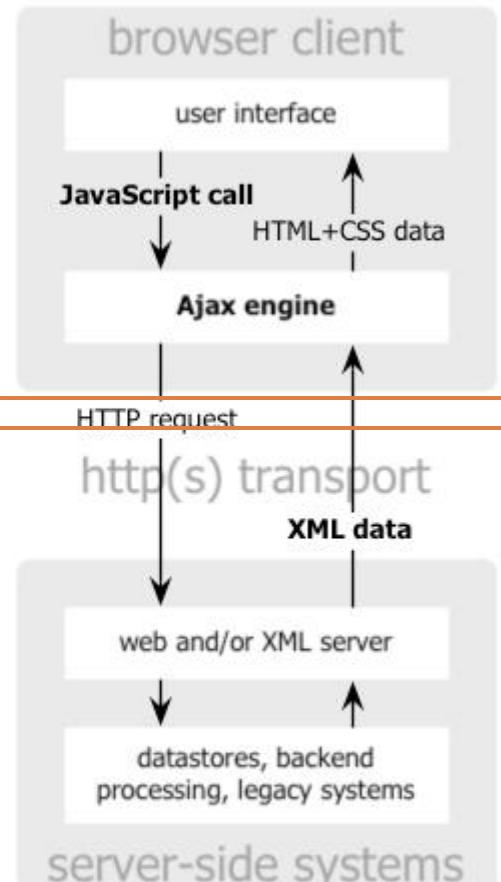
Migration Modeling Automation

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Specific client as TOMATE



classic
web application model



Ajax
web application model

SFPP3

- As a framework with reusable design, SFPP3 will be used to develop and glue together the different components of TOMATE (Tri Layer Optimized Engine) in support of the EU project Migresives.

OLD APPLICATION IN SFPP3

http://localhost/home/Diffusion_1DFVnx.sfpp3.html

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INPUT FORM

■ GETTING STARTED ■ NOTATIONS ■ INPUTS ■ FORM ■ 3D>1D MODELER ■ FV MONOLAYER ■ FV PERMEATION ■

QSPR-MS WEB-SERVER
THE CURRENT APPLICATION IS CONNECTED WITH THE EU/FP6/MIGRESIVE PROJECT

MULTILAYER MATERIALS
QSPR-MS

1D DESORPTION SIMULATION
Compliance testing emphasis

The standard 2nd degree finite element method is still available for comparison.
Advanced users: >>How to take a decision with different sources of uncertainty
Related tool: >>FV MONOLAYER simulation

NOTATIONS

INPUTS

PARAMETER FORM

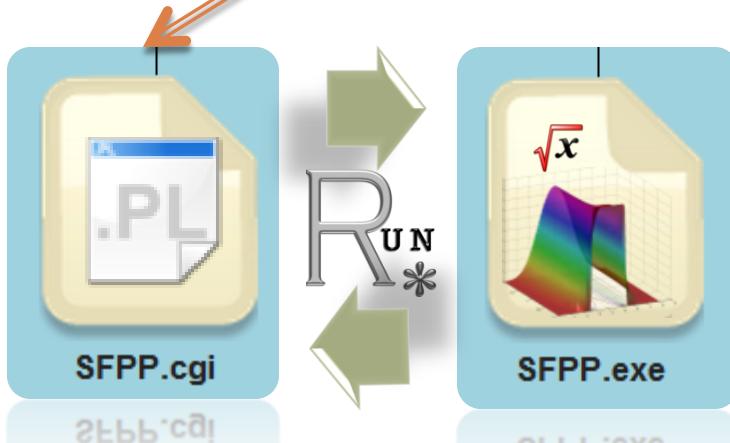
add layer delete layer TIPS‡ Order: _F=Food, _P1=layer in contact with food To remove a layer: assign its length to 0 or delete it

static form

| parameter | unit | _F | _P1 | _P2 | _P3 |
|--------------|--|------|-------|-------|-------|
| <i>l</i> | μm | - | 50 | 20 | 50 |
| <i>L_FPt</i> | kgF kgP-1 | 9 | - | - | - |
| <i>rho</i> | kg m^{-3} or g cm^{-3} | 1 | 1 | 1 | 1 |
| <i>k</i> | variable | 1 | 1 | 1 | 1 |
| <i>Dt</i> | $\text{m}^2 \text{s}^{-1}$ | - | 1e-14 | 1e-14 | 1e-14 |
| <i>Bi</i> | none | 1000 | - | - | - |
| <i>C0‡</i> | ppm | - | 500 | 500 | 500 |
| <i>t</i> | days | 10 | - | - | - |

Save parameters Launch simulation
 << Choose here the accuracy of the solution
 "normal" is always recommended as a first guess.
 Results are open in a new window

©2007 by INRA/Olivier Vitrac



OLD APPLICATION IN SFPP3

http://localhost/home/Diffusion_1DFVnx.sfpp3.html

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RESULT FORM

Inputs and outputs summary

| Properties | Assigned values |
|--|---|
| ASSUMPTIONS | nlayers=3 1D desorption/one side contact (left) no swelling/plasticizing/blooming effects Henry isotherms |
| MESH QUALITY | normal |
| DILUTION FACTOR | L_FP=9 |
| GEOMETRIES | L_P = [50 20 50] μm |
| DENSITIES | rho/rho0 = [1 1 1] |
| INITIAL CONCENTRATIONS | C_P0 = [500 500 500] ppm |
| HENRY LIKE COEFFICIENTS | k/k0 = [1 1 1] |
| DIFFUSION COEFFICIENTS | D_P = [1e-014 1e-014 1e-014] m ² .s ⁻¹ |
| DIMENSIONLESS EXTERNAL MASS TRANSPORT RESISTANCE | Bi=h.lref/Dref=1000 (reference layer = #1) |
| TIME/DIMENSIONLESS TIME | t=10 days; Fo=Dref.t/lref ² =3.456 (reference layer = #1) |
| REQUESTED CONCENTRATION IN FOOD OR SIMULANT | C_F=42.1 ppm |
| EXPECTED CONCENTRATION IN FOOD/SIMULANT AT EQUILIBRIUM | C_F_eq=50 ppm |
| time to reach 90% of C_F_eq | 13 days |
| time to reach 75% of C_F_eq | 7.2 days |
| time to reach 50% of C_F_eq | 2.9 days |
| time to reach 25% of C_F_eq | 1.7 hours |
| time to reach 10% of C_F_eq | 2.6 hours |
| time to reach 5% of C_F_eq | 40 minutes |
| time to reach 1% of C_F_eq | 2.9 minutes |
| SOLVER INFORMATION | CPU=2.27 s; solver="diffusion_1DFVn" host="127.0.0.1" |

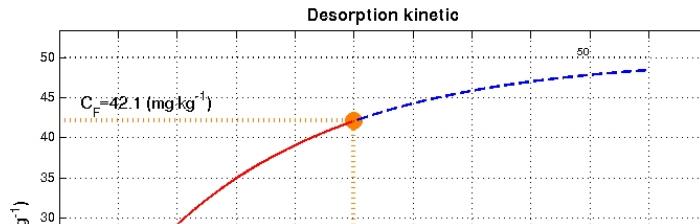


my.SFPP3.html

Export results (including figures)

[>>> EXCEL™ file <<<](#) [>>> PDF document <<<](#)

Figures



Inputs and outputs summary

| Properties | Assigned values |
|--|---|
| assumptions | nlayers=3 1D desorption/one side contact (left) no swelling/plasticizing/blooming effects Henry isotherms |
| dilution factor | L_FP=9 |
| geometries | L_P = [50 20 50] μm |
| densities | rho/rho0 = [1 1 1] |
| initial concentrations | C_P0 = [500 500 500] ppm |
| dimensionless external mass transport resistance | Bi=h.lref/Dref=1000 (reference layer = #1) |
| requested concentration in food or simulant | C_F=42.1 ppm |
| expected concentration in food/simulant at equilibrium | C_F_eq=50 ppm |
| time to reach 90% of C_F_eq | 13 days |
| time to reach 75% of C_F_eq | 7.2 days |
| time to reach 50% of C_F_eq | 2.9 days |
| time to reach 25% of C_F_eq | 1.7 hours |
| time to reach 10% of C_F_eq | 2.6 hours |
| time to reach 5% of C_F_eq | 40 minutes |
| time to reach 1% of C_F_eq | 2.9 minutes |
| solver information | CPU=2.27 s; solver="diffusion_1DFVn" host="127.0.0.1" |

Export results (including figures)

[>>> EXCEL™ file <<<](#) [>>> PDF document <<<](#)

Figures

Desorption kinetic

Safe Packaging Portal™ : http://h29.univ-reims.fr/

Results are provided: AS IS

desorption: http://h29.univ-reims.fr/desorption.html
date: 2009-01-21 02:21:20 - Jan 2009 21:52:32.499000+0000
host: SFPP3

Inputs and outputs summary

| Properties | Assigned values |
|--|---|
| assumptions | nlayers=3 1D desorption/one side contact (left) no swelling/plasticizing/blooming effects Henry isotherms |
| dilution factor | L_FP=9 |
| geometries | L_P = [50 20 50] μm |
| densities | rho/rho0 = [1 1 1] |
| initial concentrations | C_P0 = [500 500 500] ppm |
| henry like coefficients | k/k0 = [1 1 1] |
| diffusion coefficients | D_P = [1e-014 1e-014 1e-014] m ² .s ⁻¹ |
| dimensionless external mass transport resistance | Bi=h.lref/Dref=1000 (reference layer = #1) |
| time/dimensionless time | t=10 days; Fo=Dref.t/lref ² =3.456 (reference layer = #1) |
| requested concentration in food or simulant | C_F=42.1 ppm |
| expected concentration in food/simulant at equilibrium | C_F_eq=50 ppm |
| time to reach 90% of C_F_eq | 13 days |
| time to reach 75% of C_F_eq | 7.2 days |
| time to reach 50% of C_F_eq | 2.9 days |
| time to reach 25% of C_F_eq | 1.7 hours |
| time to reach 10% of C_F_eq | 2.6 hours |
| time to reach 5% of C_F_eq | 40 minutes |
| time to reach 1% of C_F_eq | 2.9 minutes |
| solver information | CPU=2.27 s; solver="diffusion_1DFVn" host="127.0.0.1" |

kinetic in F

profile in P



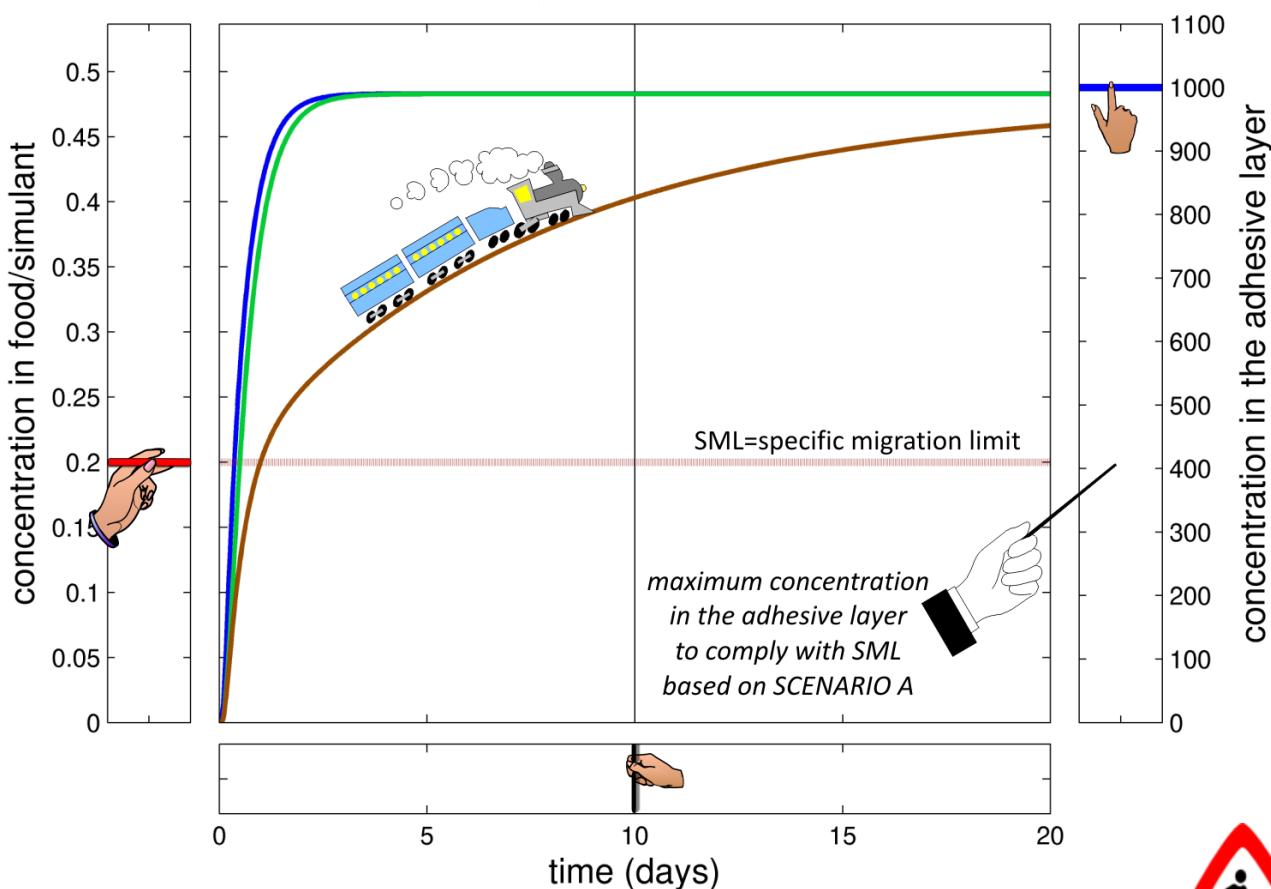
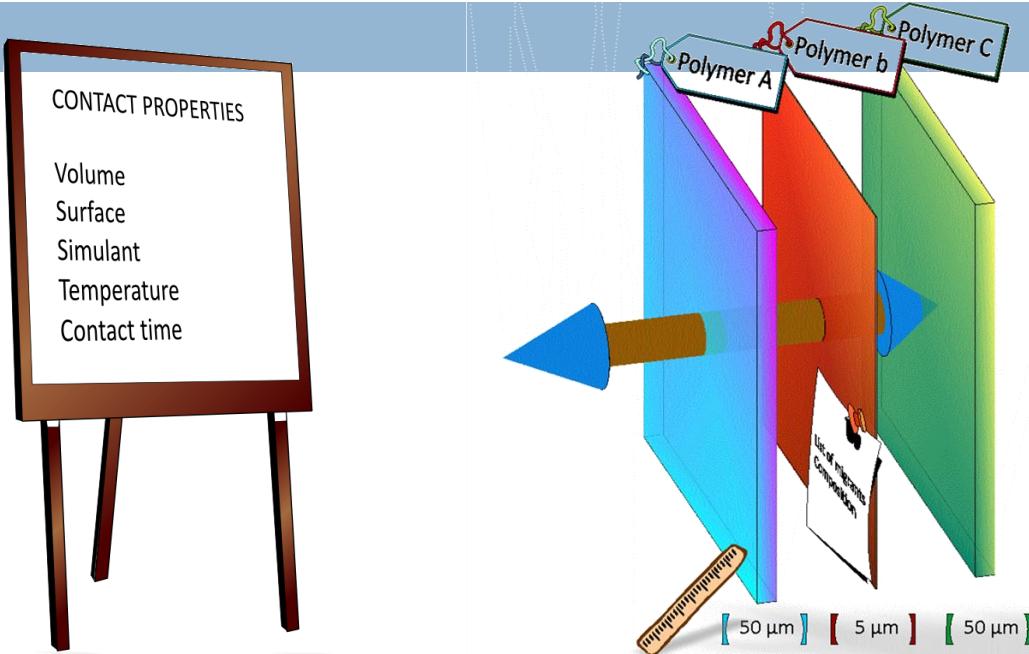
Desorption kinetic

NEW SFPP3 APPLICATION

Tri-layer Optimized MATerial Engine



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REQUEST-BUILDER

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Tools to manage your simulated results: view, export, delete

■ installed SFPP3 applications ■ input files ■ archives ■ home/ ■

SFPP3-XML-RESULTS request helper for AJAX/SPRY™ file=QSPR_arc2009.xml

Use this tool to create automatic request to saved results in JAVASCRIPT.

This interface allows you to set the values to create, validate and visualize a Spry XML request on SFPP3 data.

The information you will use to create the data set/subset will be the same as the data entered here.

For GET, enter a relative path to the XML file you wish to parse. By default, the field is set to explore an XML file we included in the download of Spry. For POST, set the URL and the POST Data. Change the content type if needed. POST data is formatted as usual: file=myresult.xml&prop=myprop. The Data Set Constructor code will show you the exact code needed to produce the displayed data set.

1. Set the SFPP3 request parameters, your file result, then hit the "Load SFPP3 Results" button:

| | |
|---------------------------|--|
| method: | GET |
| url: | /cgi-bin/output.cgi?file=QSPR_arc2009.xml |
| postData: | file=QSPR_arc2009.xml |
| Content-type: | application/x-www-form-urlencoded; charset=UTF-8 |
| useCache: | <input checked="" type="checkbox"/> |
| Load SFPP3 Results | |

2. Click on a Results list item, in the area below, to generate a data subset:

- @size
- @type
- arc
 - @idx
 - @size
 - @type
 - id (REPEATING NODE)
 - @idx
 - @size
 - @type
 - caller (REPEATING NODE)
 - @idx
 - @size
 - @type
 - date (REPEATING NODE)

3. Details (note that some Browsers remove large data sets):

XPath: /opt/arc/file

Data Set Constructor Code:

```
var dsData = new Spry.Data.XMLDataSet("/cgi-bin/output.cgi?file=QSPR_arc2009.xml", "/opt/arc/file");
```

| @idx | @size | @type | file | ds_RowID | ds_XMLNode |
|------|-------|-------|--|----------|------------------|
| 1 | 1 40 | char | diffusion_1DVFn_26-Jan-2009_12-54-46.xml | 0 | [object Element] |
| 2 | 1 40 | char | diffusion_1DVFn_26-Jan-2009_12-56-28.xml | 1 | [object Element] |
| 3 | 1 40 | char | diffusion_1DVFn_26-Jan-2009_17-37-45.xml | 2 | [object Element] |
| 4 | 1 37 | char | diffusion_1D_27-Jan-2009_16-50-36.xml | 3 | [object Element] |

SAFE FOOD PACKAGING PORTAL

2009-01-28 17:23:31

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XPath: /opt/arc/file

Data Set Constructor Code:

```
var dsData = new Spry.Data.XMLDataSet("/cgi-bin/output.cgi?file=QSPR_arc2009.xml", "/opt/arc/file");
```

DATA OBJECT MODEL

LIST OF AVAILABLE RESULTS

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/home/archive/QSPR_arc2009.xml



Job 1

Job 2

Job 3

```
<!-- SFPP3\INRA-Olivier Vitrac 26-Jan-2009 17:37:51 -->
<root xml_tb_version="2.0" idx="1" type="struct" size="1 1">
  <arc idx="1" type="struct" size="1 3">
    <id idx="1" type="double" size="1 1">1</id>
    <now idx="1" type="double" size="1 1">733799.5381112732</now>
    <host idx="1" type="char" size="1 9">127.0.0.1</host>
    <caller idx="1" type="char" size="1 22">diffusion_1DFn::SFPP3</caller>
    <date idx="1" type="char" size="1 20">26-Jan-2009 12:54:52</date>
    <path idx="1" type="char" size="1 30">Q:\SFPP3\html\www\home\archive</path>
    <file idx="1" type="char" size="1 40">diffusion_1DFn_26-Jan-2009_12-54-46.xml</file>
    <id idx="2" type="double" size="1 1">2</id>
    <now idx="2" type="double" size="1 1">733799.5392807291</now>
    <host idx="2" type="char" size="1 9">127.0.0.1</host>
    <caller idx="2" type="char" size="1 22">diffusion_1DFn::SFPP3</caller>
    <date idx="2" type="char" size="1 20">26-Jan-2009 12:56:33</date>
    <path idx="2" type="char" size="1 30">Q:\SFPP3\html\www\home\archive</path>
    <file idx="2" type="char" size="1 40">diffusion_1DFn_26-Jan-2009_12-56-28.xml</file>
    <id idx="3" type="double" size="1 1">3</id>
    <now idx="3" type="double" size="1 1">733799.7345945718</now>
    <host idx="3" type="char" size="1 9">127.0.0.1</host>
    <caller idx="3" type="char" size="1 22">diffusion_1DFn::SFPP3</caller>
    <date idx="3" type="char" size="1 20">26-Jan-2009 17:37:48</date>
    <path idx="3" type="char" size="1 30">Q:\SFPP3\html\www\home\archive</path>
    <file idx="3" type="char" size="1 40">diffusion_1DFn_26-Jan-2009_17-37-45.xml</file>
  </arc>
  <alive idx="1" type="double" size="1 3">1 2 3</alive>
</root>
```

Jobs history

Never deleted

Jobs which are still alive

(which can be converted in PDF, XLS)

Current life time = 30 days

DATA OBJECT MODEL

LIST OF AVAILABLE RESULTS

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/home/archive/QSPR_arc2009.xml

Job 1

Tree View XSL Output

```

xml version="1.0"
SFPP3\INRA-Olivier Vitrac 26-Jan-2009 17:20:11

root
  xml_tb_version 2.0
  idx 1
  type struct
  size 1 1

  arc
    idx 1
    type struct
    size 1 3

    id
      idx 1
      type double
      size 1 1
      #text 1

    now
      idx 1
      type double
      size 1 1
      #text 733799.5381112732

    host
      idx 1
      type char
      size 1 9
      #text 127.0.0.1

    caller
      idx 1
      type char
      size 1 22
      #text diffusion_1DFvN::SFPP3

    date
      idx 1
      type char
      size 1 20
      #text 26-Jan-2009 12:54:52

    path
      idx 1
      type char
      size 1 30
      #text Q:\SFPP3\html\www\home\archive

    file
      idx 1
      type char
      size 1 40
      #text diffusion_1DFvN_26-Jan-2009_12-54-46.xml

    alive
      idx 1
      type double
      size 1 3
      #text 1 2 3

```

3 jobs

Numeric date and time

Server which performed calculations

SFPP3 module

Date and time

Local path

File results

Other jobs

Alive jobs



QSPR_arc2009.xml

Data Set Constructor Code:

```
var dsData = new Spry.Data.XMLDataSet("/cgi-bin/output.cgi?file=diffusion_1DVFn_26-Jan-2009_17-37-45.xml&xml=kinetics", "/opt");
```



REQUEST-BUILDER

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Tools to manage your simulated results: view, export, delete



■ Installed SFPP3 applications ■ input files ■ archives ■ home/ ■
SFPP3-XML-RESULTS request helper for AJAX/SPRY™
 file=diffusion_1DVFn_26-Jan-2009_17-37-45.xml prop=description

Use this tool to create automatic request to saved results in JAVASCRIPT.

This interface allows you to set the values to create, validate and visualize a Spry XML request on SFPP3 data.

The information you will use to create the data set/subset will be the same as the data entered here.

For GET, enter a relative path to the XML file you wish to parse. By default, the field is set to explore an XML file we included in the download of Spry. For POST, set the URL and the POST Data. Change the content type if needed. POST Data is formatted as usual: file=myresult.xml&prop=myprop. The Data Set Constructor code will show you the exact code needed to produce the displayed data set.

1. Set the SFPP3 request parameters, your file result, then hit the "Load SFPP3 Results" button:

| | |
|---------------------------|--|
| method: | GET |
| url: | /cgi-bin/output.cgi?file=diffusion_1DVFn_26-Jan-2009_17-37-45.xml&prop=description |
| postData: | file=diffusion_1DVFn_26-Jan-2009_17-37-45.xml&prop=description |
| Content-type: | application/x-www-form-urlencoded; charset=UTF-8 |
| useCache: | <input checked="" type="checkbox"/> |
| Load SFPP3 Results | |

2. Click on a Results list item, in the area below, to generate a data subset:

- opt
 - @idx
 - @size
 - @type
 - item (REPEATING NODE)
 - @idx
 - @size
 - @type

3. Details (note that some Browsers remove large data sets):

XPath: /opt/item

Data Set Constructor Code:

```
var dsData = new Spry.Data.XMLDataSet("/cgi-bin/output.cgi?file=diffusion_1DVFn_26-Jan-2009_17-37-45.xml&xml=description", "/opt/item");
```

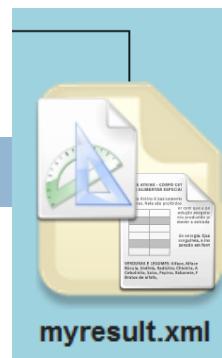
| @idx | @size | @type | item | ds_RowID | ds_XMLNode |
|------|-------|-------|---|----------|------------------|
| 1 | 1 10 | char | Properties | 0 | [object Element] |
| 2 | 1 11 | char | ASSUMPTIONS | 1 | [object Element] |
| 3 | 1 12 | char | MESH QUALITY | 2 | [object Element] |
| 4 | 1 15 | char | DILUTION FACTOR | 3 | [object Element] |
| 5 | 1 10 | char | GEOMETRIES | 4 | [object Element] |
| 6 | 1 9 | char | DENSITIES | 5 | [object Element] |
| 7 | 1 22 | char | INITIAL CONCENTRATIONS | 6 | [object Element] |
| 8 | 1 23 | char | HENRY LIKE COEFFICIENTS | 7 | [object Element] |
| 9 | 1 22 | char | DIFFUSION COEFFICIENTS | 8 | [object Element] |
| 10 | 1 48 | char | DIMENSIONLESS EXTERNAL MASS TRANSPORT RESISTANCE | 9 | [object Element] |
| 11 | 1 23 | char | TIME/DIMENSIONLESS TIME | 10 | [object Element] |
| 12 | 1 43 | char | REQUESTED CONCENTRATION IN FOOD OR SIMULANT | 11 | [object Element] |
| 13 | 1 54 | char | EXPECTED CONCENTRATION IN FOOD/SIMULANT AT EQUILIBRIUM | 12 | [object Element] |
| 14 | 1 27 | char | time to reach 90% of C_F_eq | 13 | [object Element] |
| 15 | 1 27 | char | time to reach 75% of C_F_eq | 14 | [object Element] |
| 16 | 1 27 | char | time to reach 50% of C_F_eq | 15 | [object Element] |
| 17 | 1 27 | char | time to reach 25% of C_F_eq | 16 | [object Element] |
| 18 | 1 27 | char | time to reach 10% of C_F_eq | 17 | [object Element] |
| 19 | 1 26 | char | time to reach 5% of C_F_eq | 18 | [object Element] |
| 20 | 1 26 | char | time to reach 1% of C_F_eq | 19 | [object Element] |
| 21 | 1 18 | char | SOLVER INFORMATION | 20 | [object Element] |
| 22 | 1 15 | char | Assigned values | 21 | [object Element] |
| 23 | 1 105 | char | nlayers=3 1D desorption/one side contact (left) no swelling/plasticizing/blooming effects Henry isotherms | 22 | [object Element] |
| 24 | 1 6 | char | normal | 23 | [object Element] |
| 25 | 1 6 | char | L_FP=9 | 24 | [object Element] |
| 26 | 1 22 | char | L_P = [50 20 100] um | 25 | [object Element] |
| 27 | 1 21 | char | rho/rho0 = [1 1 1] | 26 | [object Element] |
| 28 | 1 24 | char | C_P0 = [500 500 0] ppm | 27 | [object Element] |
| 29 | 1 17 | char | k/k0 = [1 1 1] | 28 | [object Element] |
| 30 | 1 37 | char | D_P = [1e-014 1e-014 1e-012] m^2 s^-1 | 29 | [object Element] |

DATA OBJECT MODEL

RESULT FILE

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/home/archive/diffusion_1DVFn_26-Jan-2009_17-37-45.xml



DEBUG TOOLS

to track bug and misconfigurations

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<http://localhost/cgi-bin/error.cgi?&debug>

- [installed SFFP3 applications](#) ■ [input files](#) ■ [archives](#) ■ [home/](#) ■ [help](#) ■

SFPP3 DEBUG MODE

Review your jobs and SFPP3 configuration.

PROBLEM

10 of 10

- 1) review your job or similar jobs ([search your job\(s\) here](#))
 - 2) restart the simulation

The problem occurred after you launch a calculation

- 3) if you can reproduce the problem, download the job as an XML file
 - 4) if there is an intermediate result, download it as an XML file ([search results here](#))
 - 5) e-mail corresponding XML file(s) to [Olivier Vitrac](#)

The problem is related to a configuration problem

- 1) Check that %SYSTEMDRIVE%\SFPP3\MCR\78 is in your PATH
 - 2) Check that %SYSTEMDRIVE%\SFPP3\Perl\bin is in your PATH
 - 3) Read the installation documentation located in %SYSTEMDRIVE%\SFPP3\readme.txt
 - 4) Run the setup.exe located in %SYSTEMDRIVE%\SFPP3\Setup\ to install SFPP3

Note that most scripts features or sim

Note that most scripts/features of simulation tools may have generated warnings or error messages before producing any valid HTML.

SOLUTION

- 1) review your job or similar jobs ([search your job\(s\) here](#))
 - 2) restart the simulation
 - 3) if you can reproduce the problem, download the job as XML
 - 4) if there is an intermediate result, download it as an XML
 - 5) e-mail corresponding XML file(s) to [Olivier Vitrac](#)

- 1) Check that %SYSTEMDRIVE%\SFPP3\MCR\v78 is in your PATH
- 2) Check that %SYSTEMDRIVE%\SFPP3\Perl\bin is in your PATH
- 3) Read the installation documentation located in %SYSTEMDRIVE%\SFPP3\readme.txt
- 4) Read the architecture documentation located in %SYSTEMDRIVE%\SFPP3\architecture.txt

- 1) Extract the last lines of error log ([click here to view the error log](#))
- 2) Check last requests to the server ([click here to view the access log](#))
- 3) Look for intermediate results (e.g. graphs) in temp directory ([click here to view the site map](#))
local path to tmp: %SYSTEMDRIVE%\SFPP3\html\www\tmp\
- 4) Please contact the SFPP3 standalone/server administrator,
Member Services and inform them of the time the error occurred,
and anything you might have done that may have caused the error.

As a rule of thumb, print this page as useful information is included in the footer

2009-02-01 11:06:40 on WSLP-Olivier2(192.168.0.16)MSWin32 <5.008007>
SAFE FOOD PACKAGING PORTAL ©INRA\Olivier Vitrac

DEBUG TOOLS

to track bug and misconfigurations

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<http://localhost/cgi-bin/error.cgi?&debug>

■ installed SFPP3 applications ■ input files ■ archives ■ home/ ■ help ■

SFPP3 DEBUG MODE
Review your jobs and SFPP3 configuration.

| PROBLEM | Suggested workaround | SOLUTION |
|--|---|--|
| The problem occurred after you launch a calculation | 1) review your job or similar jobs (search your job(s) here) 2) restart the simulation 3) If you can't reproduce the problem, download the job as an XML file (the result is an intermediate result, download it as an XML file (search results here)) 5) e-mail corresponding XML file(s) to Olivier Vitrac | 1) Check that \$SYSTEMDRIVE%\SFPP3\MCR\%N% is in your PATH 2) Please make sure that \$SYSTEMDRIVE%\SFPP3Perl\Perl is in your PATH 3) Read the architecture documentation located in \$SYSTEMDRIVE%\SFPP3\architecture.txt 4) Read the architecture documentation located in \$SYSTEMDRIVE%\SFPP3\architecture.txt 1) Extract the last lines of error log (click here to view the error log) 2) If you require more information, click here to view the access log 3) Look for an undefined result (e.g. "Unknown") in the error log (Click here to view the site map) local path to top: \$SYSTEMDRIVE%\SFPP3\html\www\tmp 4) Please contact the SFPP3 standalone server administrator. Member Services and inform them of the time the error occurred, and anything you might have done that may have caused the error. |
| The problem is related to a configuration problem | | |
| Get more information of this error | | |
| Note that most scripts, failure or simulation tools may have generated warnings or error messages before producing any valid HTML. | | |

As a rule of thumb, print this page as useful information is included in the footer

2009-02-01 11:06:49 SFPP3 version 2009-01-31 23:54:38 SFPP3 version v5.80007>
SAFE FOOD PACKAGING PORTAL ©INRA/Olivier Vitrac

| List of environment variables (to be used to track misconfigurations) | |
|---|---|
| KEYWORD | VALUE |
| COMSPEC | C:\Windows\system32\cmd.exe |
| DOCUMENT_ROOT | Q:/SFPP3/html/www/ |
| GATEWAY_INTERFACE | CGI/1.1 |
| HTTP_ACCEPT | text/html,application/xhtml+xml,application/xml;q=0.9,*/*;q=0.8 |
| HTTP_ACCEPT_CHARSET | ISO-8859-1,utf-8;q=0.7,*;q=0.7 |
| HTTP_ACCEPT_ENCODING | gzip,deflate |
| HTTP_ACCEPT_LANGUAGE | fr,fr;q=0.8,en-us;q=0.5,en;q=0.3 |
| HTTP_CONNECTION | keep-alive |
| HTTP_HOST | 127.0.0.1 |
| HTTP_KEEP_ALIVE | 300 |
| HTTP_USER_AGENT | Mozilla/5.0 (Windows; U; Windows NT 6.0; fr; rv:1.9.0.5) Gecko/2008120122 Firefox/3.0. |
| PATH | [MATLAB PATH] C:\MATLAB\R2008a\bin [MATLAB PATH] C:\MATLAB\R2008a\bin\win32 [MATLAB PATH] C:\MATLAB\R2007b\bin [MATLAB PATH] C:\MATLAB\R2007b\bin\win32 c:\program files\microsoft network monitor 3\ c:\cygwin\bin C:\Windows\System32\WindowsPowerShell\v1.0\ C:\Program Files\Cepstral\bin C:\Program Files\QuickTime\QTSystem\ C:\Program Files\gs\gs8.63\bin\ C:\Program Files\Common Files\Nero\Lib |

| | |
|------------------|--|
| PATHEXT | .COM;.EXE;.BAT;.CMD;.VBS;.VBE;.JS;.JSE;.WSF;.WSH;.MSC;.PY;.PYW |
| QUERY_STRING | &debug |
| REMOTE_ADDR | 127.0.0.1 |
| REMOTE_PORT | 50047 |
| REQUEST_METHOD | GET |
| REQUEST_URI | /cgi-bin/error.cgi?&debug |
| SCRIPT_FILENAME | Q:/SFPP3/html/www/cgi-bin/error.cgi |
| SCRIPT_NAME | /cgi-bin/error.cgi |
| SERVER_ADDR | 127.0.0.1 |
| SERVER_ADMIN | olivier.vitrac@agroparistech.fr |
| SERVER_NAME | 127.0.0.1 |
| SERVER_PORT | 80 |
| SERVER_PROTOCOL | HTTP/1.1 |
| SERVER_SIGNATURE | Apache/2.0.54 (Win32) mod_perl/2.0.1 Perl/v5.8.7 Server at 127.0.0.1 Port 80 |
| SERVER_SOFTWARE | Apache/2.0.54 (Win32) mod_perl/2.0.1 Perl/v5.8.7 |
| SYSTEMROOT | C:\Windows |
| WINDIR | C:\Windows |

■ installed SFPP3 applications ■ input files ■ archives ■ home/ ■ help ■

SFPP3 site map of 127.0.0.1

2009-02-01 11:13:21

Directories: 17 | ASCII: 131 | Binary: 397 | Files: 528 | Total Size: 38763 Kb.

| | |
|----------------|--|
| .No Extension: | 1 .cgi: 11 .css: 7 .db: 2 |
| .gif: | 117 .html: 19 .ico: 3 .jpeg: 26 .jpg: 46 |
| .js: | 53 .opj: 1 .pdf: 2 .pl: 1 .png: 200 |
| .txt: | 2 .xls: 2 .xml: 35 |

• /

- 1. /favicon.ico
- 2. /readme.txt

• /cgi-bin

- 1. /cgi-bin/SFPP3.cgi
- 2. /cgi-bin/SFPP3.cgi
- 3. /cgi-bin/XMLhelper.cgi
- 4. /cgi-bin/delete.cgi
- 5. /cgi-bin/error.cgi
- 6. /cgi-bin/errorlog.cgi
- 7. /cgi-bin/favicon.ico
- 8. /cgi-bin/index.cgi
- 9. /cgi-bin/input.cgi
- 10. /cgi-bin/output.cgi
- 11. /cgi-bin/plots.cgi
- 12. /cgi-bin/run.cgi
- 13. /cgi-bin/stitemap.cgi

• /cgi-bin/infile

- 1. /cgi-bin/infile/SFPP 2009-01-24 23-30-53-3522.infile.xml
- 2. /cgi-bin/infile/SFPP 2009-01-24 23-39-03-2552.infile.xml
- 3. /cgi-bin/infile/SFPP 2009-01-25 16-52-10-8749.infile.xml
- 4. /cgi-bin/infile/SFPP 2009-01-25 16-54-48-7774.infile.xml
- 5. /cgi-bin/infile/SFPP 2009-01-25 19-45-25-8588.infile.xml
- 6. /cgi-bin/infile/SFPP 2009-01-25 19-53-25-8588.infile.xml
- 7. /cgi-bin/infile/SFPP 2009-01-25 20-52-27-5908.infile.xml
- 8. /cgi-bin/infile/SFPP 2009-01-26 11-54-32-7015.infile.xml
- 9. /cgi-bin/infile/SFPP 2009-01-26 11-55-40-5920.infile.xml
- 10. /cgi-bin/infile/SFPP 2009-01-26 11-56-21-5360.infile.xml
- 11. /cgi-bin/infile/SFPP 2009-01-26 11-57-00-5930.infile.xml
- 12. /cgi-bin/infile/SFPP 2009-01-26 16-37-30-2287.infile.xml
- 13. /cgi-bin/infile/SFPP 2009-01-26 16-38-16-8579.infile.xml
- 14. /cgi-bin/infile/SFPP 2009-01-27 15-50-19-7456.infile.xml
- 15. /cgi-bin/infile/SFPP 2009-01-27 15-59-09-6613.infile.xml
- 16. /cgi-bin/infile/SFPP 2009-01-27 15-59-39-3348.infile.xml
- 17. /cgi-bin/infile/SFPP 2009-01-27 16-09-02-2740.infile.xml
- 18. /cgi-bin/infile/SFPP 2009-01-27 16-09-40-5322.infile.xml
- 19. /cgi-bin/infile/SFPP 2009-01-27 16-11-07-2862.infile.xml
- 20. /cgi-bin/infile/SFPP 2009-01-29 17-11-09-3780.infile.xml
- 21. /cgi-bin/infile/SFPP 2009-01-30 23-40-48-3186.infile.xml
- 22. /cgi-bin/infile/SFPP 2009-01-31 23-54-38-1656.infile.xml

• /css

- 1. /css/SpryAccordion.css
- 2. /css/SpryToolTips.css
- 3. /css/calc.css
- 4. /css/calendar.css
- 5. /css/flotr.css
- 6. /css/index.html
- 7. /css/main.css
- 8. /css/packaging.jpg
- 9. /css/samples.css

• /css/_notes

- 1. /css/_notes/dvSync.xml

• /help

- 1. /help/readme.txt

• /help/SFPP3_quick_start

- 1. /help/SFPP3_quick_start/SFPP3_quick_start.pdf
- 2. /help/SFPP3_quick_start/SFPP3_quick_start01.jpg
- 3. /help/SFPP3_quick_start/SFPP3_quick_start02.jpg
- 4. /help/SFPP3_quick_start/SFPP3_quick_start03.jpg
- 5. /help/SFPP3_quick_start/SFPP3_quick_start04.jpg
- 6. /help/SFPP3_quick_start/SFPP3_quick_start05.jpg
- 7. /help/SFPP3_quick_start/SFPP3_quick_start06.jpg
- 8. /help/SFPP3_quick_start/SFPP3_quick_start07.jpg
- 9. /help/SFPP3_quick_start/SFPP3_quick_start08.jpg
- 10. /help/SFPP3_quick_start/SFPP3_quick_start09.jpg
- 11. /help/SFPP3_quick_start/SFPP3_quick_start10.jpg
- 12. /help/SFPP3_quick_start/SFPP3_quick_start11.jpg
- 13. /help/SFPP3_quick_start/SFPP3_quick_start12.jpg
- 14. /help/SFPP3_quick_start/SFPP3_quick_start13.jpg
- 15. /help/SFPP3_quick_start/SFPP3_quick_start14.jpg
- 16. /help/SFPP3_quick_start/SFPP3_quick_start15.jpg
- 17. /help/SFPP3_quick_start/SFPP3_quick_start16.jpg
- 18. /help/SFPP3_quick_start/SFPP3_quick_start17.jpg
- 19. /help/SFPP3_quick_start/SFPP3_quick_start18.jpg
- 20. /help/SFPP3_quick_start/SFPP3_quick_start19.jpg
- 21. /help/SFPP3_quick_start/TBN_SFPP2_quick_start01.jpg
- 22. /help/SFPP3_quick_start/TBN_SFPP2_quick_start02.jpg
- 23. /help/SFPP3_quick_start/TBN_SFPP3_quick_start03.jpg
- 24. /help/SFPP3_quick_start/TBN_SFPP3_quick_start04.jpg
- 25. /help/SFPP3_quick_start/TBN_SFPP3_quick_start05.jpg
- 26. /help/SFPP3_quick_start/TBN_SFPP3.quick_start06.jpg
- 27. /help/SFPP3.quick_start/TBN_SFPP3.quick_start07.jpg
- 28. /help/SFPP3.quick_start/TBN_SFPP3.quick_start08.jpg
- 29. /help/SFPP3.quick_start/TBN_SFPP3.quick_start09.jpg
- 30. /help/SFPP3.quick_start/TBN_SFPP3.quick_start10.jpg
- 31. /help/SFPP3.quick_start/TBN_SFPP3.quick_start11.jpg
- 32. /help/SFPP3.quick_start/TBN_SFPP3.quick_start12.jpg