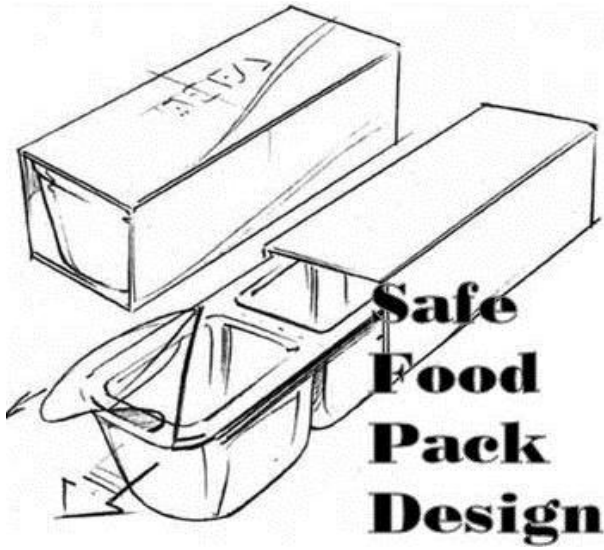
FMECAENGINE

a seamless tool to chain migration simulations and perform related sensitivity analysis

Version 0.45

(Windows & Linux i386/x64)

olivier.vitrac@agroparistech.fr



SUPPORTED BY ANR

August, 2011

LICENSE

FMECAengine is developed by Olivier Vitrac, PhD (Institut National de la Recherche Agronomique) and distributed under licence CeCILL-B (compatible GPL) as detailed below.

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http://www.cecill.info/licences/Licence_CeCILL-B_V1-en.html

Notice

This Agreement is a Free Software license agreement that is the result of discussions between its authors in order to ensure compliance with the two main principles guiding its drafting:

- firstly, compliance with the principles governing the distribution of Free Software: access to source code, broad rights granted to users,
- secondly, the election of a governing law, French law, with which it is conformant, both as regards the law of torts and intellectual property law, and the protection that it offers to both authors and holders of the economic rights over software.

GOALS

- **FMECAengine implements FMECA concepts** (http://en.wikipedia.org/wiki/FMECA) while being compatible with the underlying physics of mass transfer between food packaging and food.
- **a formalism as an expert system** that enables the simulation of various migration scenarios and the coupling with heterogeneous databases, rulebases and knwoledge bases from industry, final users, research laboratory…
- **Possible scopes**: identification of critical steps within a food packaging flow chart (setoff, hot filling, long term storage, household heating…); seeking critical migrants for various designs (e.g. from adhesives, inks); concurrent design of complex food packaging systems (multicomponents, multilayers).

VERSION HISTORY

- Generating migration scenarios (version 0.1)
- Simulating chained scenarios (version 0.2)
- Sensitivity analysis (version 0.3)
- Severity and criticality analysis (version 0.38)
- Connecting with physico-chemical databases (version 0.41)
- Multiple keys enabled in versions 0.43 and later

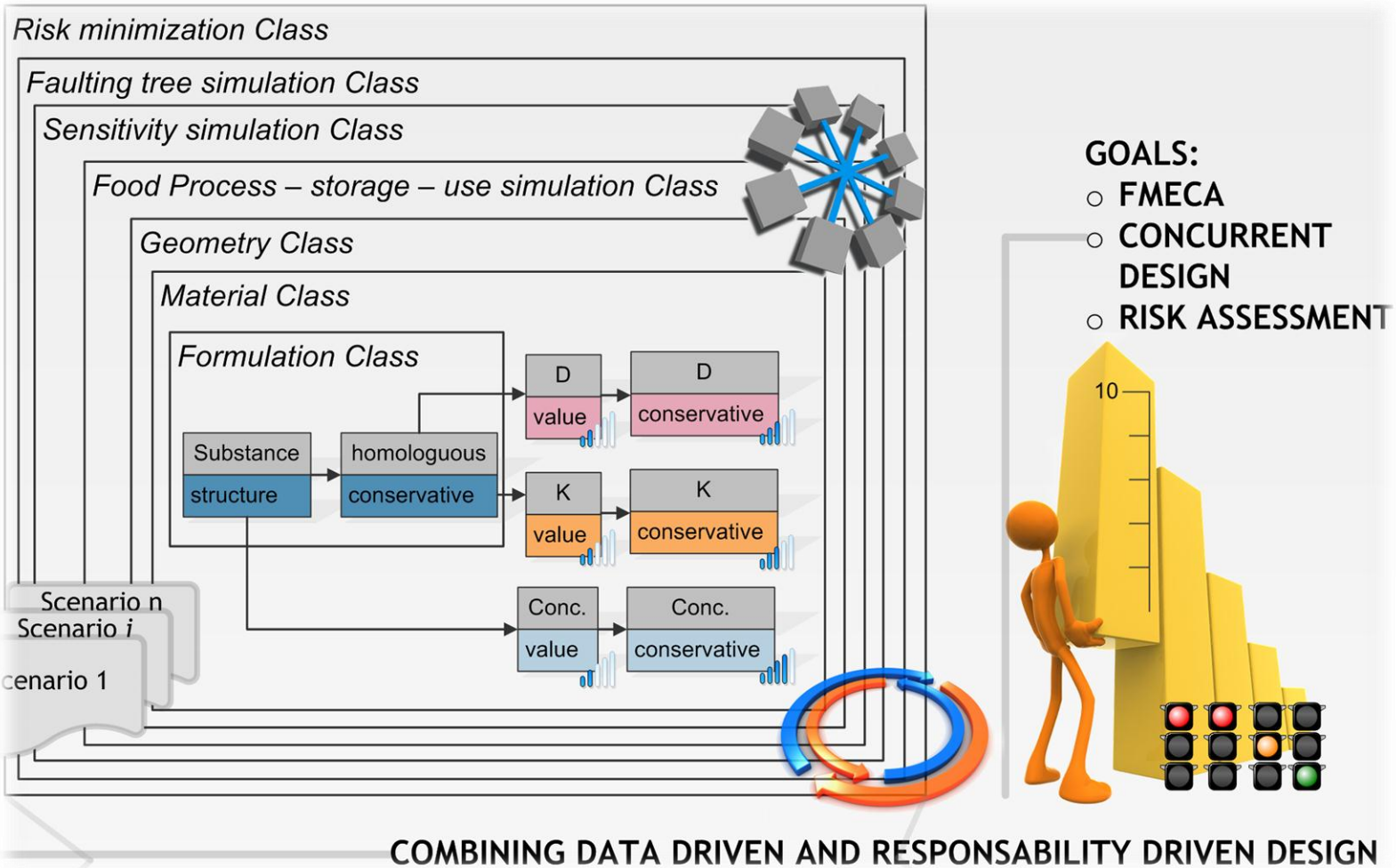
Which kind of problem can be solved ?

Setoff

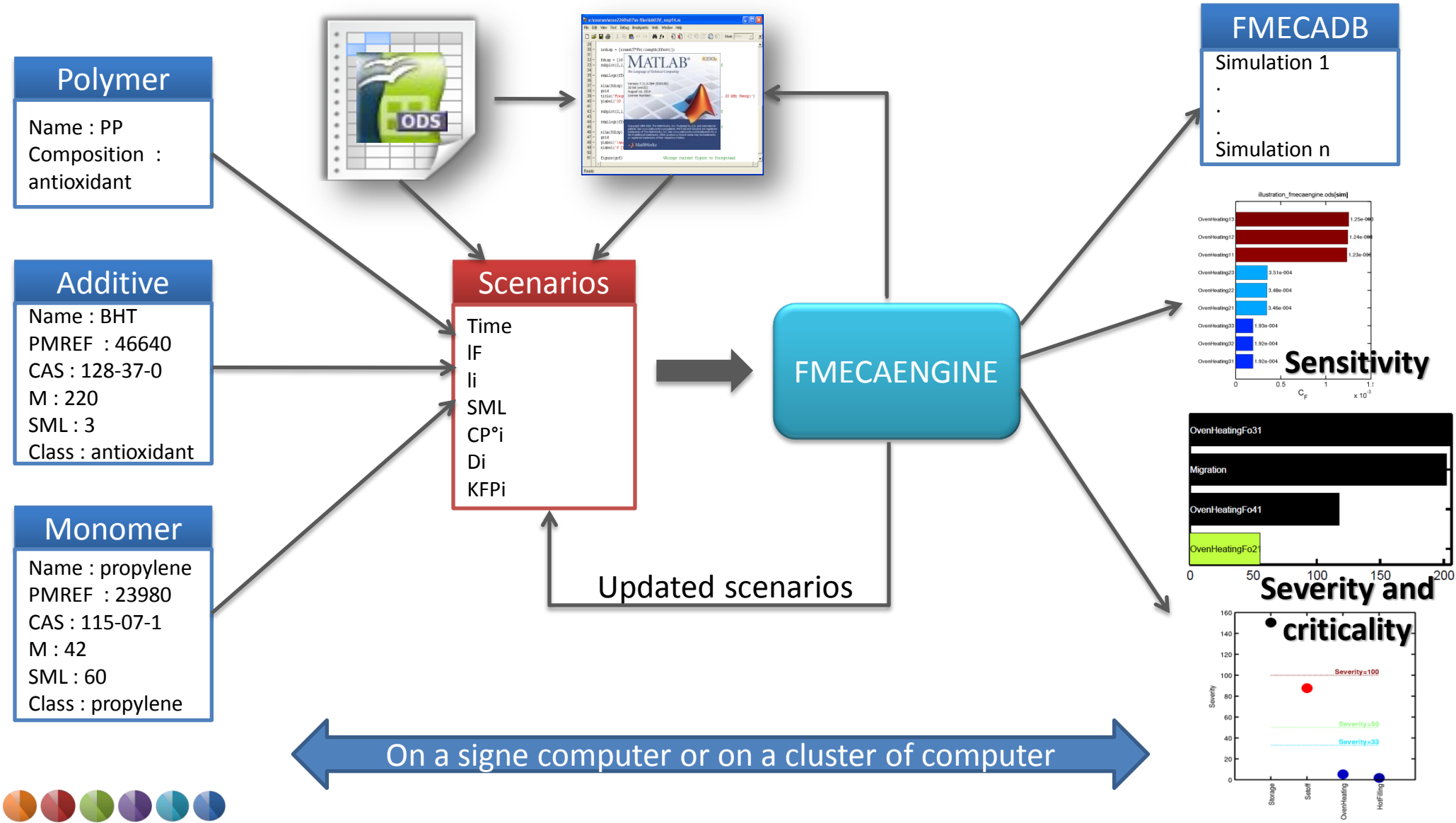
HotFilling

Storage

OvenHeating



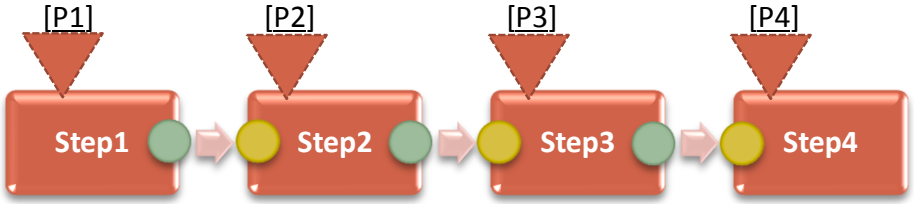
FMECAENGINE architecture



WHAT IS CHAINED SIMULATION ?

Principles : inherited parameters, parental bond

Toy example

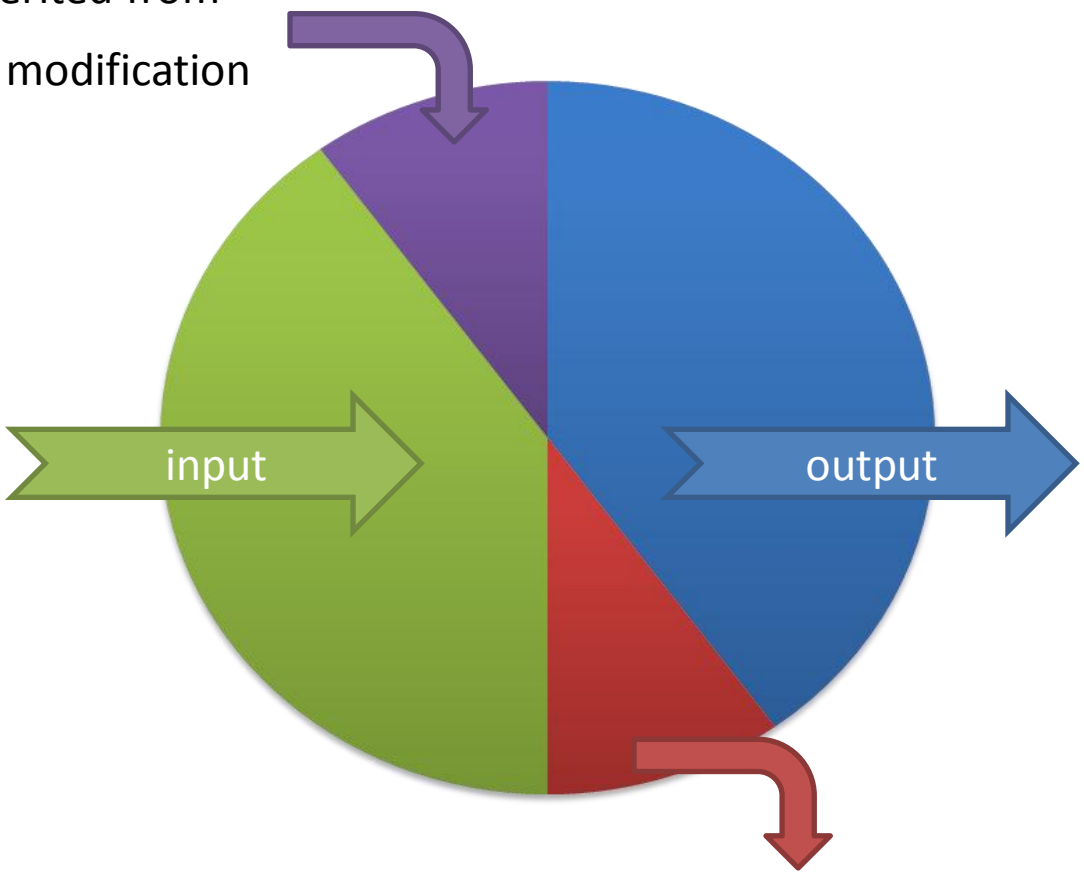


What is migration simulation?

Parameter vector inherited from step k $[\underline{p}]_k$ + sparse modification $[\underline{\delta p}]_n$

Result from a previous simulation

(e.g. time x space concentration field denoted $[\underline{\underline{c}}]_{n-1}$)



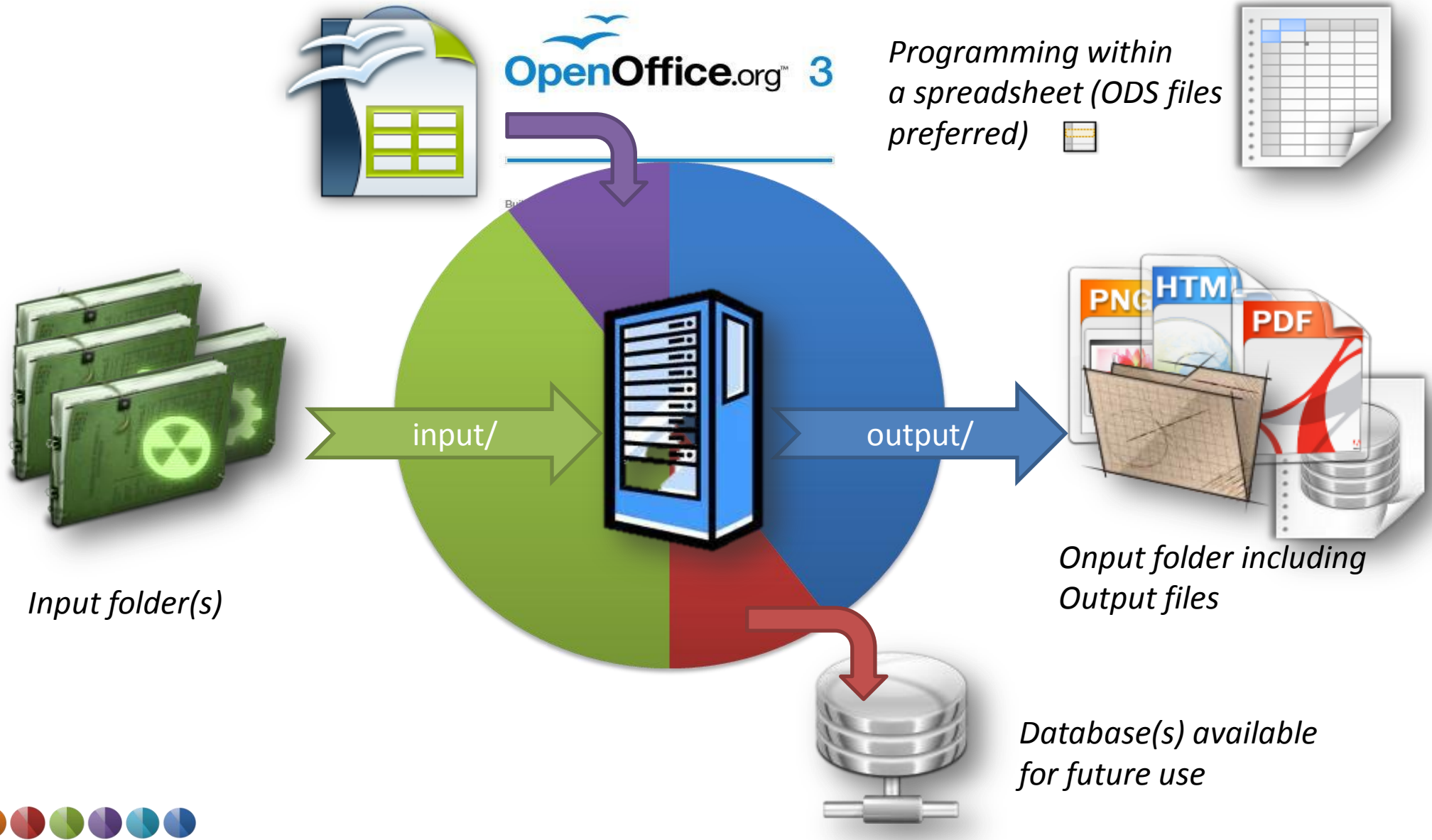
Simulated result

(denoted $[\underline{\underline{c}}]_n$)

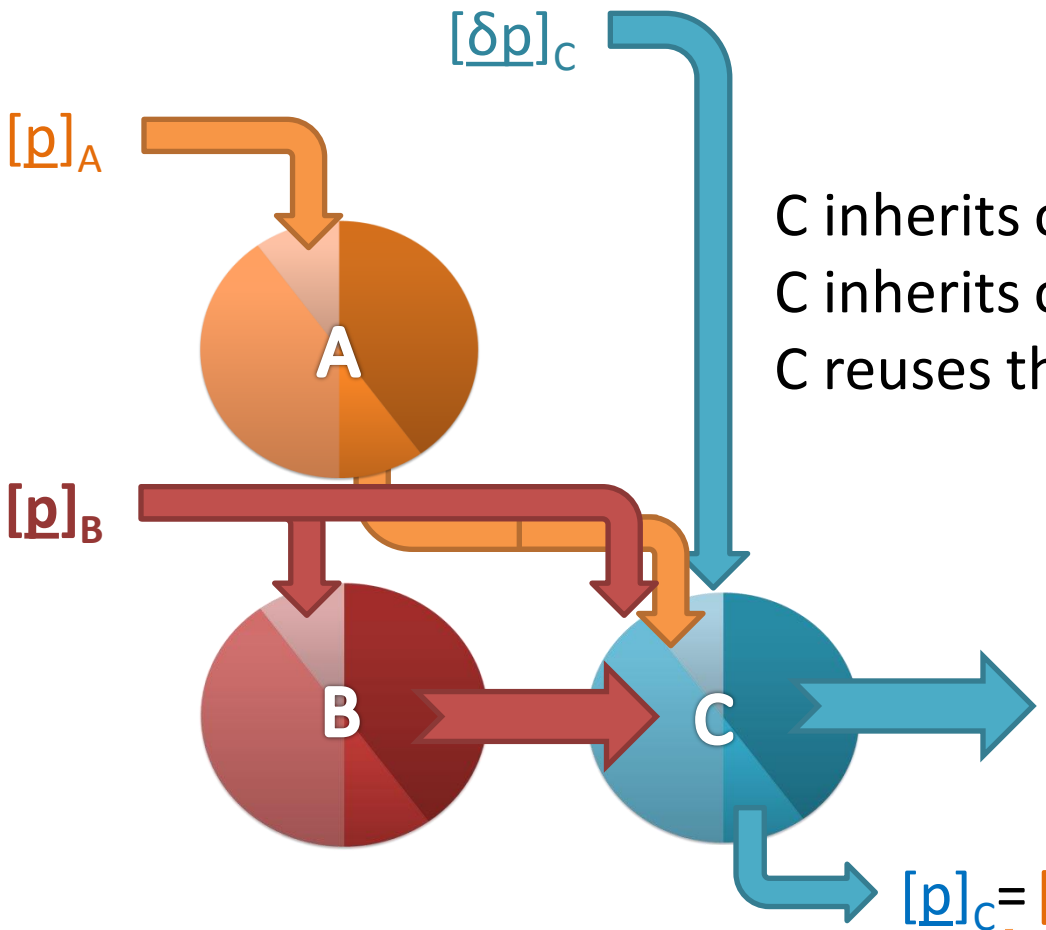
$[\underline{p}]_n = [\underline{p}]_k + [\underline{\delta p}]_n$

to propagate inheritance

Object/parallel implementation



GOAL: solve complex simulation scenarios with simple inheritance operators and sparse parameters



C inherits of parameters of A

C inherits of parameters of B

C reuses the output of B (B is the parent of C)

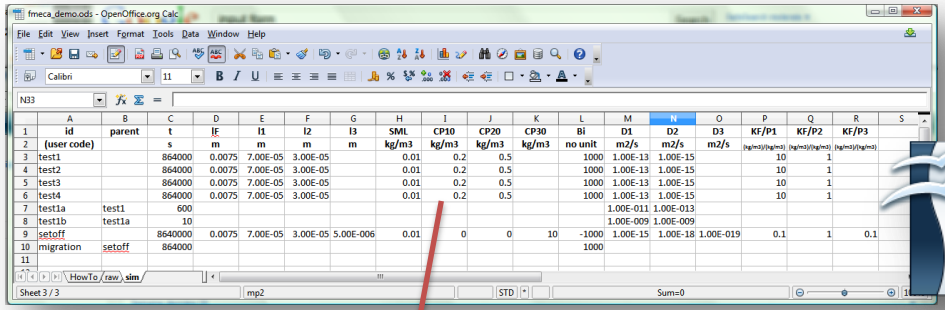
$[\underline{c}]_C = f_C([\underline{p}]_C)$

$[\underline{p}]_C = \underbrace{\mathbf{[\underline{p}]_A} + [\underline{p}]_B}_{} + [\underline{\delta p}]_C$

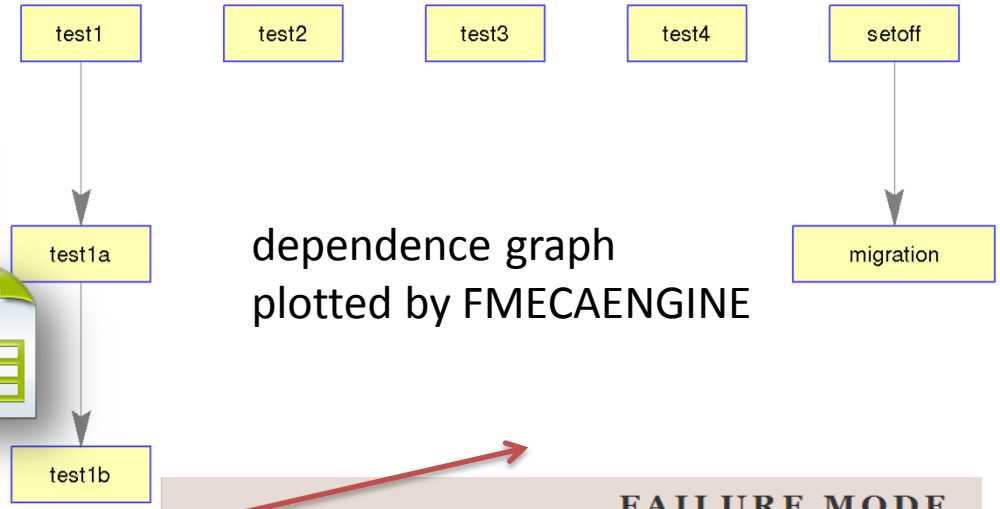
Bold=higher precedence

TOY EXAMPLE: input table

INPUT TABLE =OpenOffice worksheet (ODS v. 3)



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	id	parent	t	lF	l1	l2	l3	SML	CP10	CP20	CP30	Bi	D1	D2	D3	KF/P1	KF/P2	KF/P3
2	(user code)		s	m	m	m	m	kg/m3	kg/m3	kg/m3	kg/m3	no unit	m2/s	m2/s	m2/s	(kg/m3)/(kg/m3)	(kg/m3)/(kg/m3)	(kg/m3)/(kg/m3)
3	test1		864000	0.0075	7.00E-05	3.00E-05		0.01	0.2	0.5		1000	1.00E-13	1.00E-15		10	1	
4	test2		864000	0.0075	7.00E-05	3.00E-05		0.01	0.2	0.5		1000	1.00E-13	1.00E-15		10	1	
5	test3		864000	0.0075	7.00E-05	3.00E-05		0.01	0.2	0.5		1000	1.00E-13	1.00E-15		10	1	
6	test4		864000	0.0075	7.00E-05	3.00E-05		0.01	0.2	0.5		1000	1.00E-13	1.00E-15		10	1	
7	test1a	test1	600										1.00E-011	1.00E-013				
8	test1b	test1a	10										1.00E-009	1.00E-009				
9	setoff		8640000	0.0075	7.00E-05	3.00E-05	5.00E-006	0.01	0	0	10	-1000	1.00E-15	1.00E-18	1.00E-019	0.1	1	0.1
10	migration	setoff	864000									1000						
11																		



dependence graph
plotted by FMECAENGINE

SAFEFOODPACK DESIGN

FAILURE MODE,
EFFECTS,
AND CRITICALITY ANALYSIS
(FMECA)

Engine="**fmecaengine**" (version **0.41**) Host="**olivier@mcr10.agroparistech.fr**" (mlm release **R2010b**) Local Path="**/home/olivier/MaiNguyen/ANR_SFPD/WP2_FMECA/demo**"
Worksheet="**sim**" Input File="**fmeca_demo.ods**" FMECA Database="**fmecamodal.mat**" Input Folder="**inputs**" Output Folder="**outputs**"
result page » dependence graph (pdf)

FMECA_DEMO.ODS | 18-APR-2011 15:46:19 | 12.3 KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SFPD/WP2_FMECA/DEMO/INPUTS

id	parent	t	l_F	l_1	l_2	l_3	SML	CP_1^0	CP_2^0	CP_3^0	Bi	D_1	D_2	D_3	KFP_1	KFP_2	KFP_3
usercode		*s*	*m*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
test1		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1	
test2		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1	
test3		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1	
test4		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1	
test1a	**test1**	600										1e-11	1e-13				
test1b	**test1a**	10										1e-09	1e-09				
setoff		8.64e+06	0.0075	7e-05	3e-05	5e-06	0.006	0	0	10	-1000	1e-15	1e-18	1e-19	0.1	1	1
migration	**setoff**	864000									1000						
INPUT TABLE	8 simulation definitions						**date**	18-May-2011 16:06:27									

ORIGINAL TABLE repainted by FMECAENGINE

TOY EXAMPLE: output table

Chaining defined via ancestors MO.ODS | 18-APR-2011 15:46:19 | 12.3 KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SFPD/WP2_FMECA/DEMO/INPUTS **Results available as links**

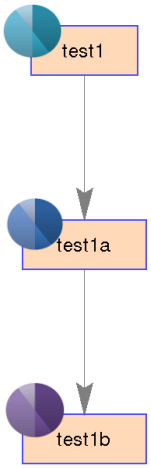
id	parent	t	l_F	l_1	l_2	l_3	SML	CP_1^0	CP_2^0	CP_3^0	Bi	D_1	D_2	D_3	KFP_1	KFP_2	KFP_3	PDF	PNG	MAT	MAT
usercode		s	m	m	m	m	kg/m³	kg/m³	kg/m³	kg/m³	no unit	m²/s	m²/s	m²/s	(kg/m³)/(kg/m³)	(kg/m³)/(kg/m³)	(kg/m³)/(kg/m³)	output	output	date	size
test1		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1		document	image	18-May-2011 16:06:37	2.2 MBytes
test2		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1		document	image	18-May-2011 16:06:29	2.2 MBytes
test3		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1		document	image	18-May-2011 16:06:30	2.2 MBytes
test4		864000	0.0075	7e-05	3e-05		0.006	0.2	0.5		1000	1e-13	1e-15		10	1		document	image	18-May-2011 16:06:31	2.2 MBytes
test1a	test1	600	~~0.0075~~	~~7e-05~~	~~3e-05~~		~~0.006~~	~~0.2~~	~~0.5~~		~~1000~~	1e-11	1e-13		~~10~~	~~1~~		document	image	18-May-2011 16:06:38	2.1 MBytes
test1b	test1a	10	~~0.0075~~	~~7e-05~~	~~3e-05~~		~~0.006~~	~~0.2~~	~~0.5~~		~~1000~~	1e-09	1e-09		~~10~~	~~1~~		document	image	18-May-2011 16:06:40	2.2 MBytes
setoff		8.64e+06	0.0075	7e-05	3e-05	5e-06	0.006	0	0	10	-1000	1e-15	1e-18	1e-19	0.1	1	0.1	document	image	18-May-2011 16:06:34	2.1 MBytes
migration	setoff	864000	~~0.0075~~	~~7e-05~~	~~3e-05~~	~~5e-06~~	~~0.006~~	~~0~~	~~0~~	~~10~~	1000	~~1e-15~~	~~1e-18~~	~~1e-19~~	~~0.1~~	~~1~~	~~0.1~~	document	image	18-May-2011 16:06:36	2.1 MBytes

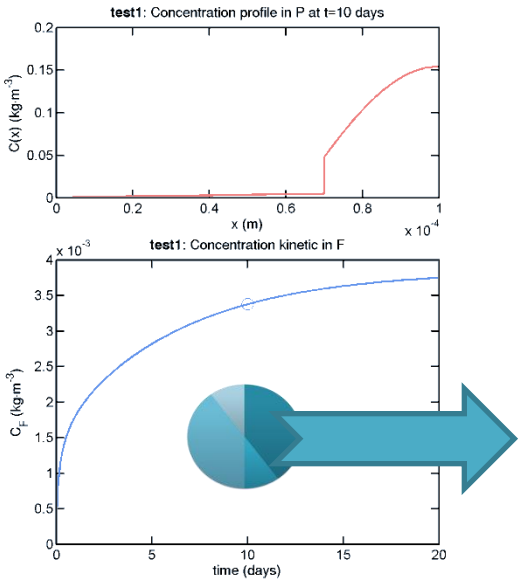
FMECA database	8 simulations	fmecamodal.mat	last update	18-May-2011 16:06:40	last report	8 simulations updated/created in 12.89 s

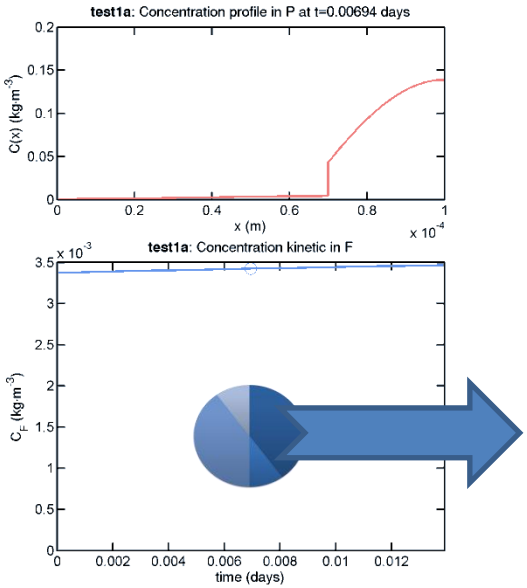
Simulations without parent are independent.

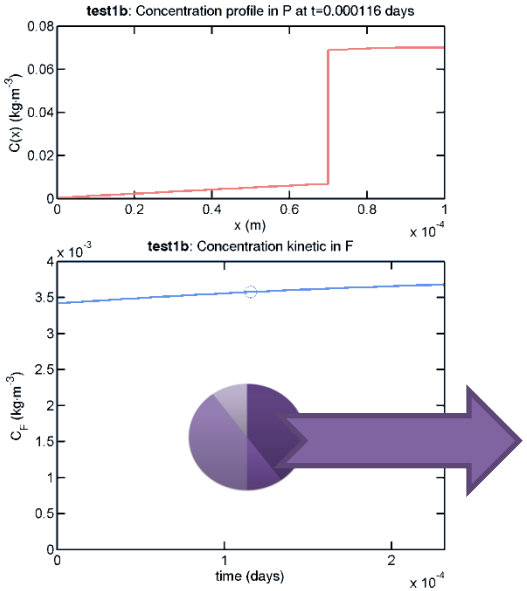
~~Line-through~~ values are inherited from their parents.

Links give direct access to plots.



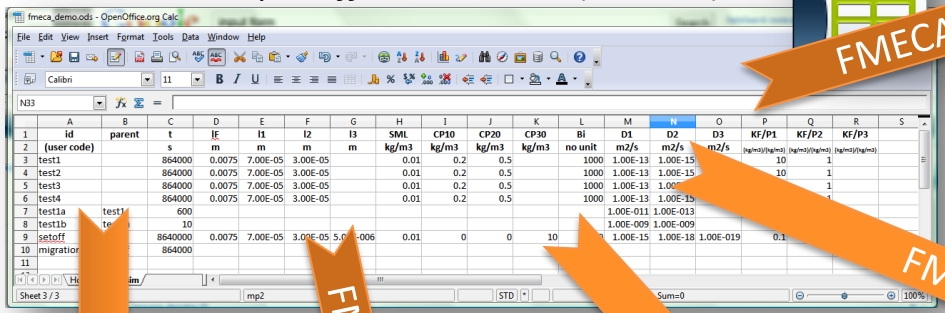




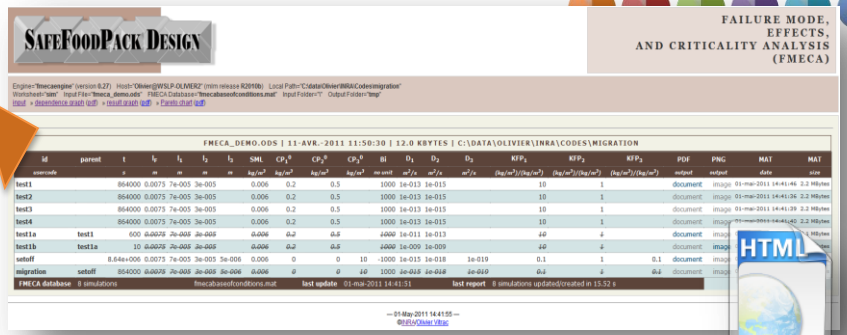


TOY EXAMPLE: outputs

INPUT TABLE =OpenOffice worksheet (ODS v. 3)

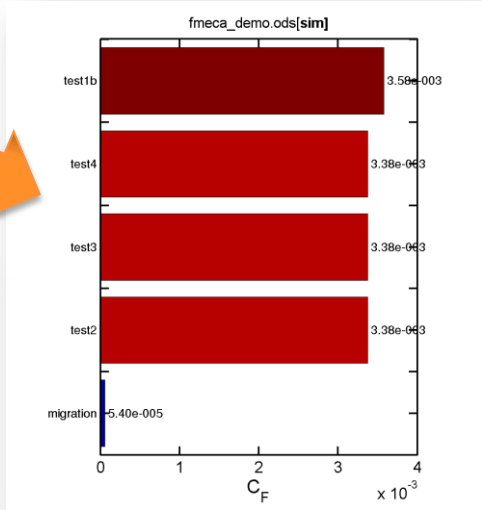


FMECAENGINE



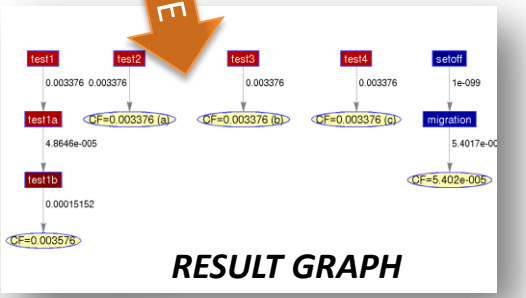
OUTPUT TABLE =HTML report

FMECAENGINE



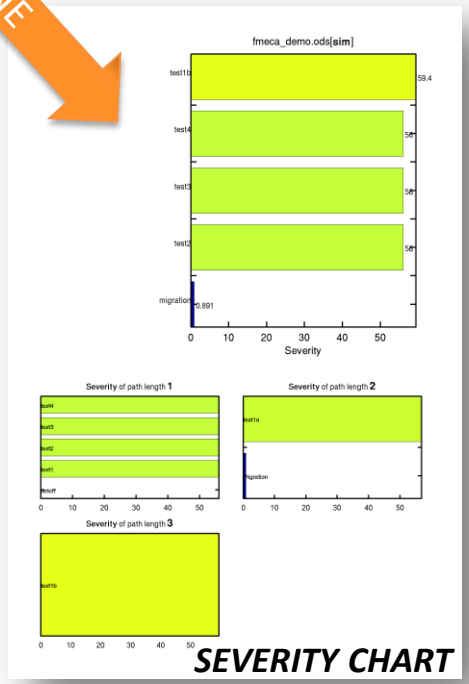
OUTPUT PARETO CHART

FMECAENGINE



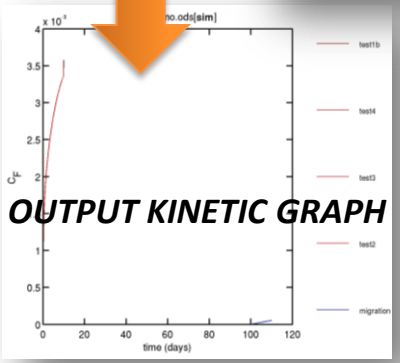
RESULT GRAPH

FMECAENGINE



SEVERITY CHART

FMECAENGINE



OUTPUT KINETIC GRAPH

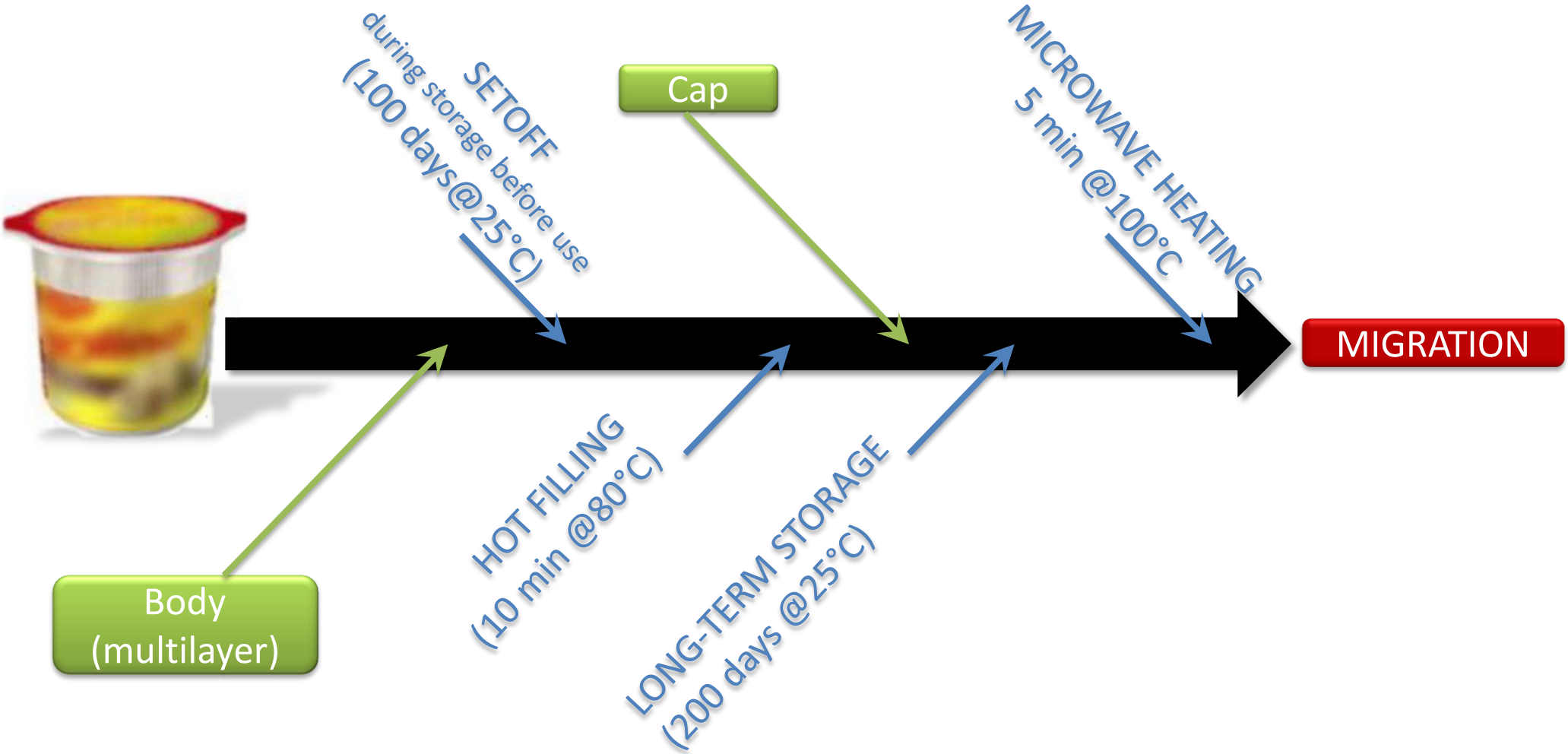
SENSIBILITY ANALYSIS

Principles : automatic creation of combinations (Foscale, Kscale)

Illustrative examples

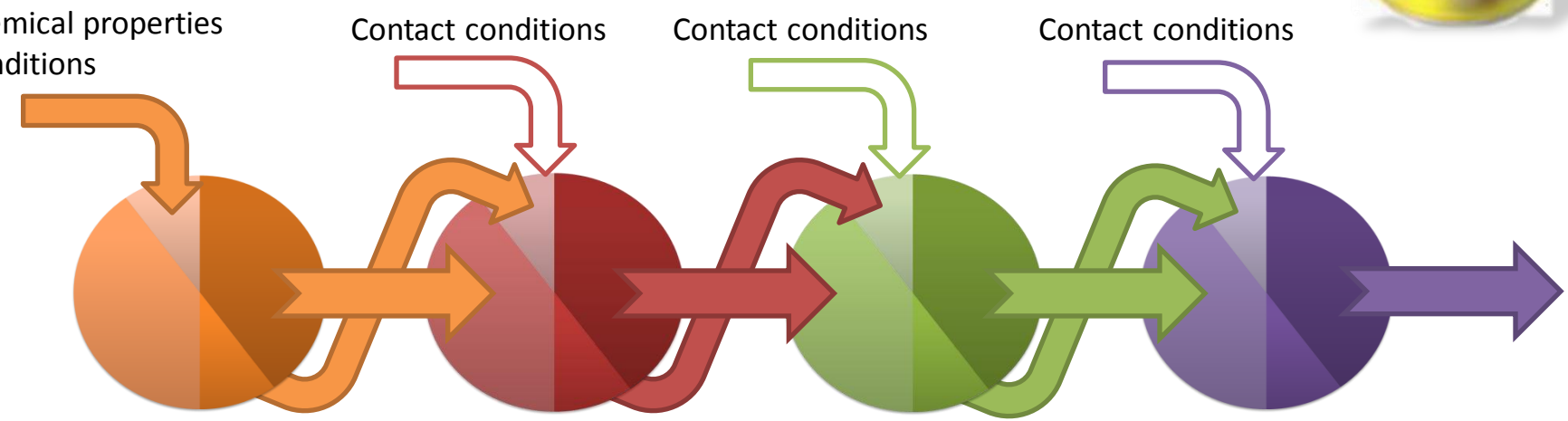
CASE STUDY

simulation chaining to assess cause trees



CORRESPONDING CODING

Geometry
Composition
Physico-chemical properties
Contact conditions



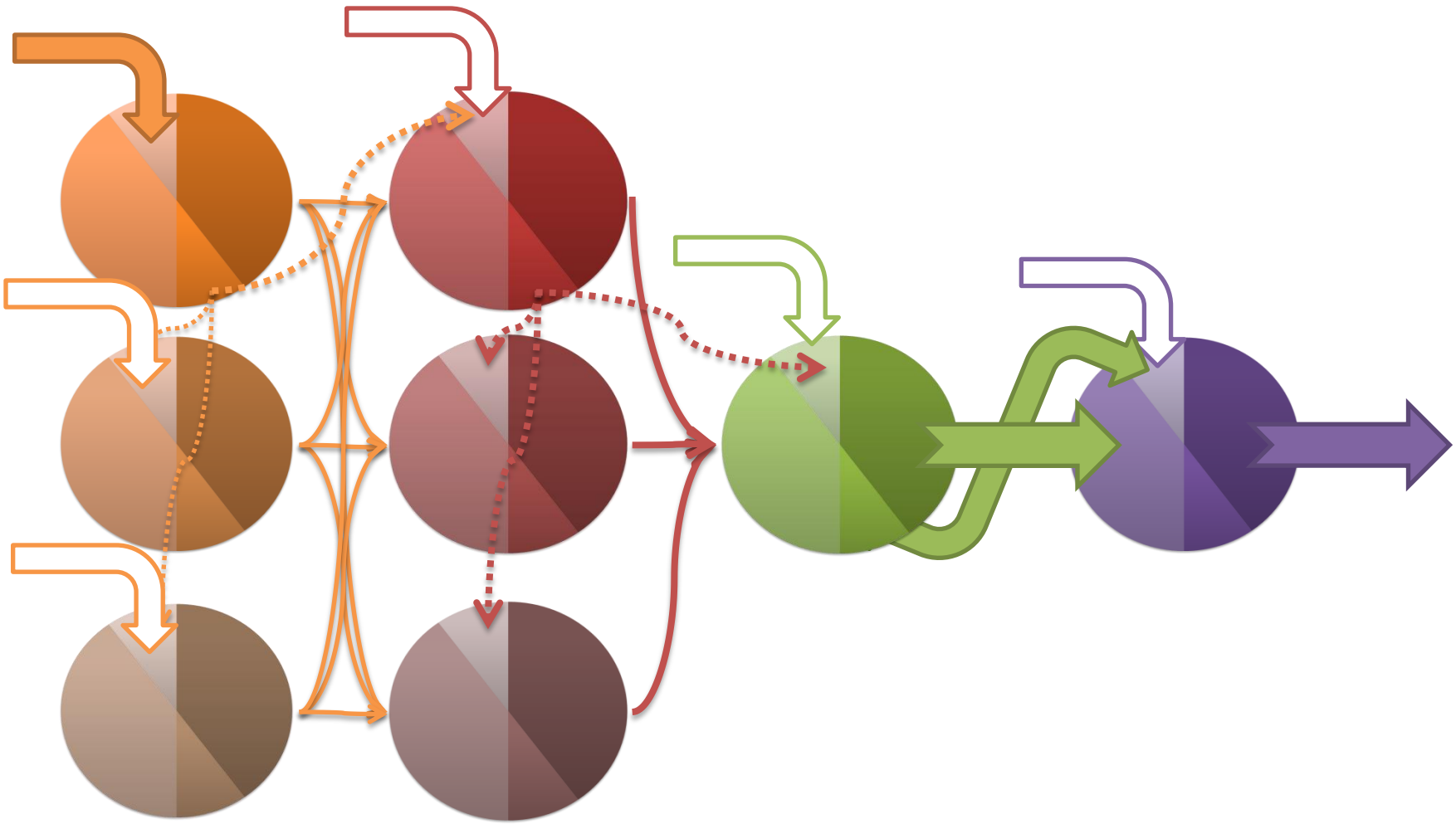
As most of values are inherited, the table is highly sparse.
Note that negative Bi values code for setoff (periodic boundary conditions).

ILLUSTRATION_FMECAENGINE.ODS | 28-AVR.-2011 22:06:43 | 23.4 KBYTES | C:\DATA\OLIVIER\INRA\ETUDIANTS & VISITEURS\AUDREY GOUJON\ILLUSTRATION_FMECA\INPUTS

row	id	parent	inherit	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	*usercode*		*inherit*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
1	**Setoff1**			8.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-014	1.2e-016	10	1
2	**HotFilling11**	**Setoff1**		600				0			1000	1.77e-011	2e-013		
3	**Storage11**	**HotFilling11**		1.728e+007				*θ*				3.3e-014	1.2e-016		
4	**OvenHeating11**	**Storage11**		300				*θ*				1.1e-010	3e-012		

SENSITIVITY OF ANALYSIS

An example: 3 levels for each first two steps



PRINCIPLES OF SENSITIVITY OF ANALYSIS

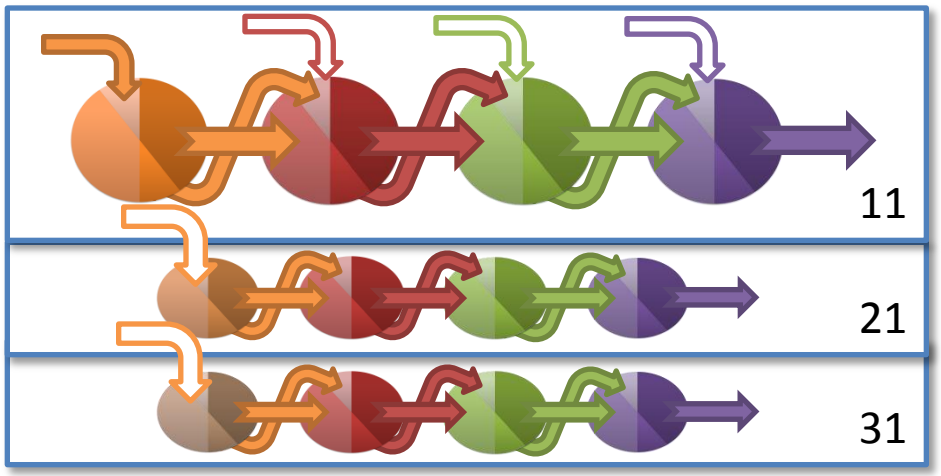
9 levels combinations

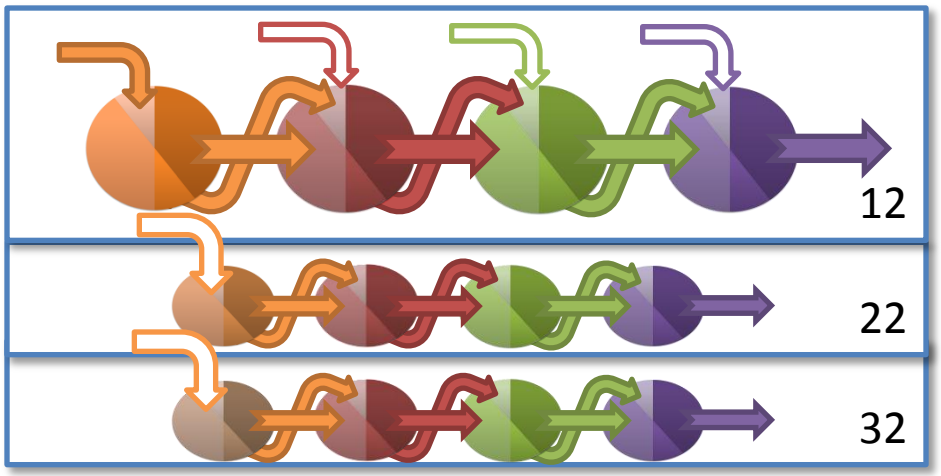
11	12	13
21	22	23
31	32	33

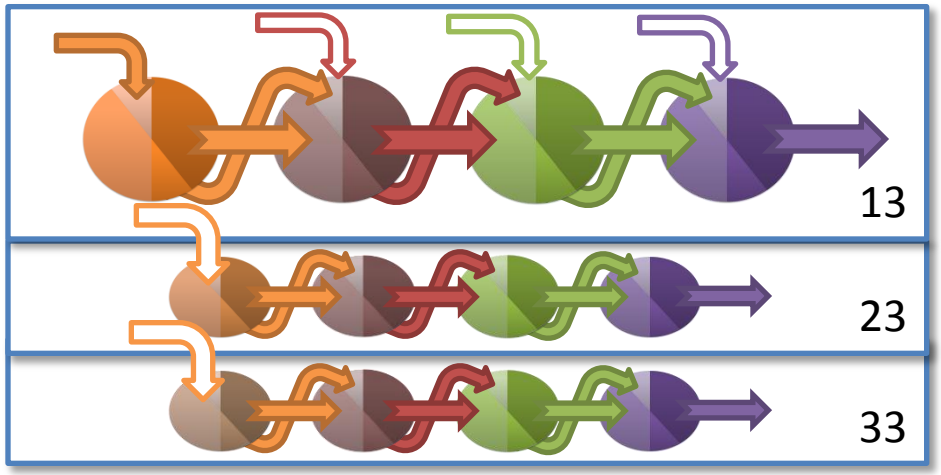
PRINCIPLES OF SENSITIVITY OF ANALYSIS

APPLICATION TO SIMULATION CHAINING

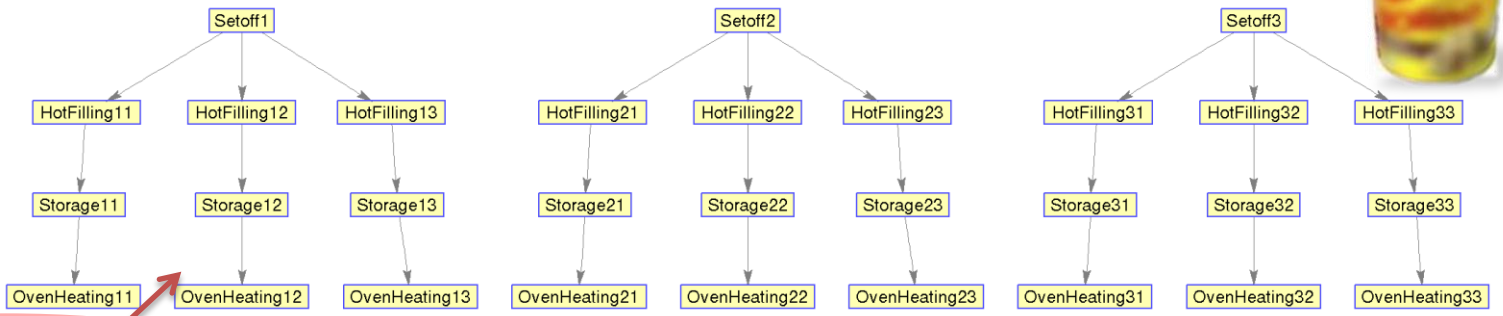
Mandatory rule = each step must have a single parent







A FIRST INTUITIVE IMPLEMENTATION: by hands



result page » dependence graph (pdf)

ILLUSTRATION_FMECAENGINE.ODS | 28-AVR.-2011 22:06:43 | 23.4 KBYTES | C:\DATA\OLIVIER\INRA\ETUDIANTS & VISITEURS\AUDREY GOUJON\ILLUSTRATION_FMECA\INPUTS

row	id	parent	inherit	t	I_F	I_1	I_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	*usercode*		*inherit*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
1	Setoff1			8.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-014	1.2e-016	10	1
2	HotFilling11	Setoff1		600				0			1000	1.77e-011	2e-013		
3	Storage11	HotFilling11		1.728e+007				θ				3.3e-014	1.2e-016		
4	OvenHeating11	Storage11		300				θ				1.1e-010	3e-012		
5	HotFilling12	Setoff1	HotFilling11	1200				θ							
6	Storage12	HotFilling12	Storage11					θ							
7	OvenHeating12	Storage12	OvenHeating11					θ							
8	HotFilling13	Setoff1	HotFilling11	1800				θ							
9	Storage13	HotFilling13	Storage11					θ							
10	OvenHeating13	Storage13	OvenHeating11					θ							
11	Setoff2		Setoff1					0				5.11e-015	3e-017		
12	HotFilling21	Setoff2	HotFilling11					θ				2.74e-012	4e-014		
13	Storage21	HotFilling21	Storage11					θ				5.11e-015	3e-017		
14	OvenHeating21	Storage21	OvenHeating11					θ				1.7e-011	2.5e-013		
15	HotFilling22	Setoff2	HotFilling21	1200				θ							
16	Storage22	HotFilling22	Storage21					θ							
17	OvenHeating22	Storage22	OvenHeating21					θ							
18	HotFilling23	Setoff2	HotFilling21	1800				θ							
19	Storage23	HotFilling23	Storage21					θ							
20	OvenHeating23	Storage23	OvenHeating21					θ							
21	Setoff3		Setoff1					0				1.33e-015	1.7e-017		
22	HotFilling31	Setoff3	HotFilling11					θ				7.11e-013	9e-015		
23	Storage31	HotFilling31	Storage11					θ				1.33e-015	1.7e-017		
24	OvenHeating31	Storage31	OvenHeating11					θ				4.41e-012	5e-014		
25	HotFilling32	Setoff3	HotFilling31	1200				θ							
26	Storage32	HotFilling32	Storage31					θ							
27	OvenHeating32	Storage32	OvenHeating31					θ							
28	HotFilling33	Setoff3	HotFilling31	1800				θ							
29	Storage33	HotFilling33	Storage31					θ							
30	OvenHeating33	Storage33	OvenHeating31					θ							

INPUT TABLE 30 simulation definitions date 30-Apr-2011 19:46:00

INTPUT TABLE

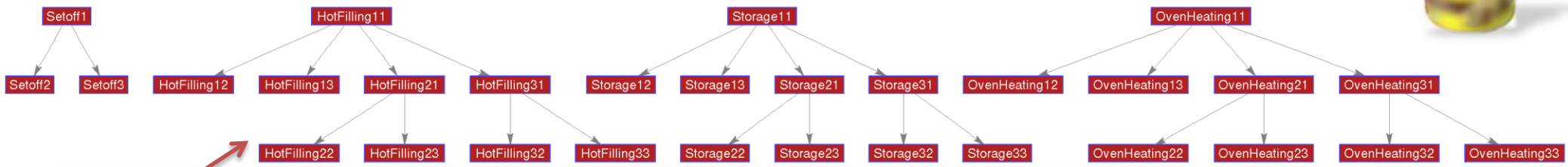
TION_FMECAENGINE.ODS | 28-AV

	id	parent	inher
	usercode		*inher*
1	Setoff1		
2	HotFilling11	Setoff1	
3	Storage11	HotFilling11	

Relationship defined with “id” and “parent”

Note the sparsity of inputs

SPARSITY: PARAMETERS ARE MAINLY INHERITED



input » dependence graph (pdf) » result graph (pdf) » Pareto chart (pdf) » Kinetics (pdf) » Severity chart (pdf)

Reconstructed full table from column "inherit"

ILLUSTRATION_FMECAENGINE.ODS | 16-MAY-2011 14:45:14 | 25.6 KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SFPD/WP2_FMECA/ILLUSTRATION_FMECA/INPUTS

row	id	parent	inherit	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2	PDF	PNG	MAT	MAT
row	*usercode*		*inherit*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*	*output*	*output*	*date*	*size*
1	Setoff1			8.64e+06	0.0115385	0.001	5e-05	0.0006	0	0.5	-1000	3.3e-14	1.2e-16	10	1	document	image	18-May-2011 15:49:56	2.0 MBytes
2	HotFilling11	Setoff1		600	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	1000	1.77e-11	2e-13	~~10~~	~~1~~	document	image	18-May-2011 15:49:57	1.9 MBytes
3	Migration11	HotFilling11		1.728e+07	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	3.3e-14	1.2e-16	~~10~~	~~1~~	document	image	18-May-2011 15:49:58	2.2 MBytes
4	OvenHeating11	Migration11		300	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	1.1e-10	3e-12	~~10~~	~~1~~	document	image	18-May-2011 15:49:59	2.0 MBytes
5	HotFilling12	Setoff1	HotFilling11	1200	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.77e-11~~	~~2e-13~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:01	2.0 MBytes
6	Migration12	HotFilling12	Migration11	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~3.3e-14~~	~~1.2e-16~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:02	2.2 MBytes
7	OvenHeating12	Migration12	OvenHeating11	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.1e-10~~	~~3e-12~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:03	2.0 MBytes
8	HotFilling13	Setoff1	HotFilling11	1800	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.77e-11~~	~~2e-13~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:04	2.0 MBytes
9	Migration13	HotFilling13	Migration11	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~3.3e-14~~	~~1.2e-16~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:05	2.2 MBytes
10	OvenHeating13	Migration13	OvenHeating11	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.1e-10~~	~~3e-12~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:06	2.0 MBytes
11	Setoff2		Setoff1	~~8.64e+06~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~-1000~~	5.11e-15	3e-17	~~10~~	~~1~~	document	image	18-May-2011 15:50:07	2.0 MBytes
12	HotFilling21	Setoff2	HotFilling11	~~600~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	2.74e-12	4e-14	~~10~~	~~1~~	document	image	18-May-2011 15:50:08	2.0 MBytes
13	Migration21	HotFilling21	Migration11	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	5.11e-15	3e-17	~~10~~	~~1~~	document	image	18-May-2011 15:50:09	2.2 MBytes
14	OvenHeating21	Migration21	OvenHeating11	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	1.7e-11	2.5e-13	~~10~~	~~1~~	document	image	18-May-2011 15:50:10	1.8 MBytes
15	HotFilling22	Setoff2	HotFilling21	1200	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~2.74e-12~~	~~4e-14~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:11	2.1 MBytes
16	Migration22	HotFilling22	Migration21	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~5.11e-15~~	~~3e-17~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:12	2.2 MBytes
17	OvenHeating22	Migration22	OvenHeating21	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.7e-11~~	~~2.5e-13~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:13	1.8 MBytes
18	HotFilling23	Setoff2	HotFilling21	1800	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~2.74e-12~~	~~4e-14~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:14	2.1 MBytes
19	Migration23	HotFilling23	Migration21	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~5.11e-15~~	~~3e-17~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:16	2.1 MBytes
20	OvenHeating23	Migration23	OvenHeating21	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.7e-11~~	~~2.5e-13~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:17	1.8 MBytes
21	Setoff3		Setoff1	~~8.64e+06~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~-1000~~	1.33e-15	1.7e-17	~~10~~	~~1~~	document	image	18-May-2011 15:50:18	2.0 MBytes
22	HotFilling31	Setoff3	HotFilling11	~~600~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	7.11e-13	9e-15	~~10~~	~~1~~	document	image	18-May-2011 15:50:19	2.0 MBytes
23	Migration31	HotFilling31	Migration11	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	1.33e-15	1.7e-17	~~10~~	~~1~~	document	image	18-May-2011 15:50:20	2.2 MBytes
24	OvenHeating31	Migration31	OvenHeating11	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	4.41e-12	5e-14	~~10~~	~~1~~	document	image	18-May-2011 15:50:21	1.9 MBytes
25	HotFilling32	Setoff3	HotFilling31	1200	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~7.11e-13~~	~~9e-15~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:22	2.1 MBytes
26	Migration32	HotFilling32	Migration31	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.33e-15~~	~~1.7e-17~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:23	2.2 MBytes
27	OvenHeating32	Migration32	OvenHeating31	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~4.41e-12~~	~~5e-14~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:24	1.9 MBytes
28	HotFilling33	Setoff3	HotFilling31	1800	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~7.11e-13~~	~~9e-15~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:25	2.1 MBytes
29	Migration33	HotFilling33	Migration31	~~1.728e+07~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~1.33e-15~~	~~1.7e-17~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:26	2.2 MBytes
30	OvenHeating33	Migration33	OvenHeating31	~~300~~	~~0.0115385~~	~~0.001~~	~~5e-05~~	~~0.0006~~	~~0~~	~~0.5~~	~~1000~~	~~4.41e-12~~	~~5e-14~~	~~10~~	~~1~~	document	image	18-May-2011 15:50:27	1.9 MBytes

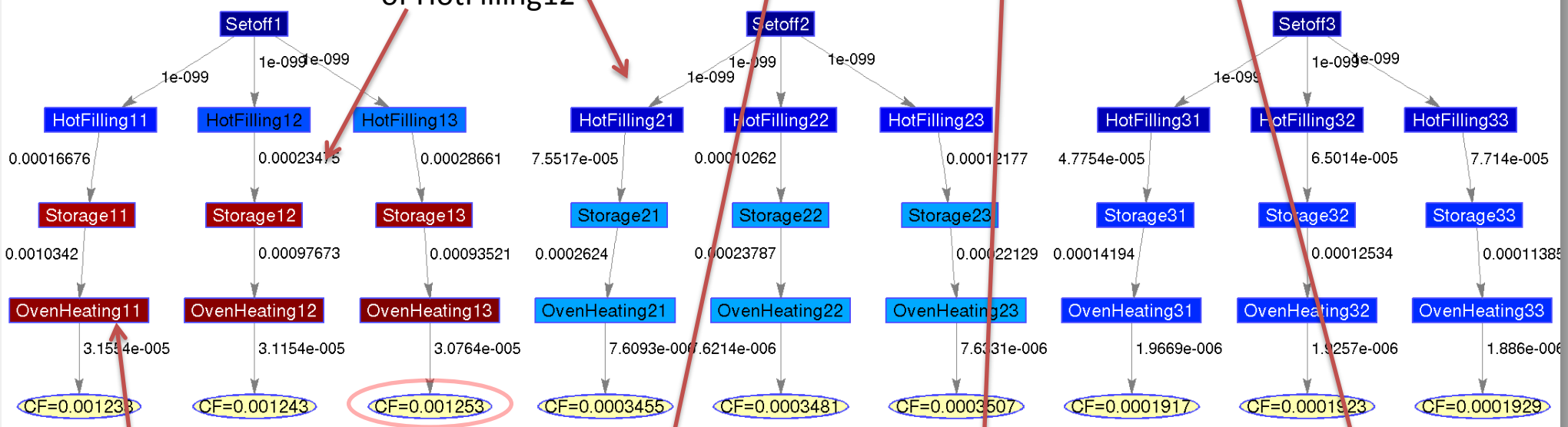
FMECA database 30 simulations fmecamodal.mat **last update** 18-May-2011 15:54:39 **last report** 0 simulations updated/created in 0.6776 s

OUTPUT TABLE

RAPID RESULTS ANALYSIS

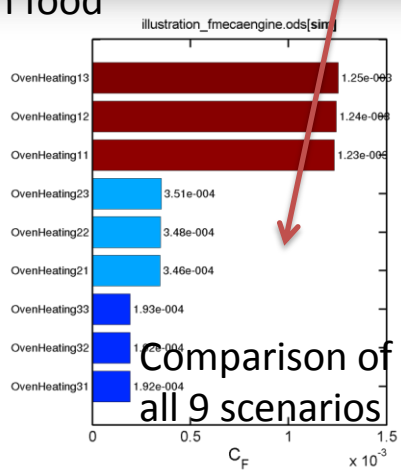
input » dependence graph (pdf) » result graph (pdf) » Pareto chart (pdf) » Kinetics (pdf) » Severity chart (pdf)

Contribution of HotFilling12

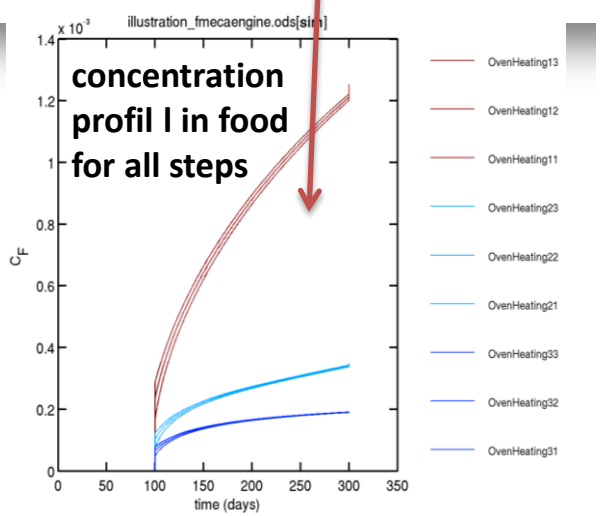


Final concentration value in food

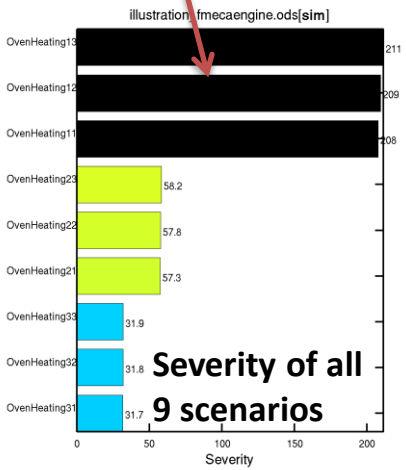
Color proportional to The concentration in food (jet colormap).



Comparison of all 9 scenarios

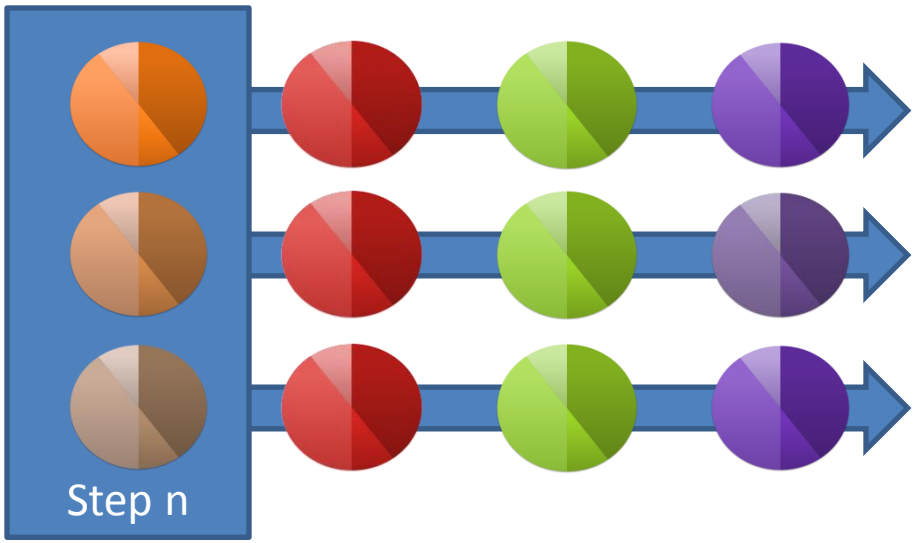


concentration profil l in food for all steps



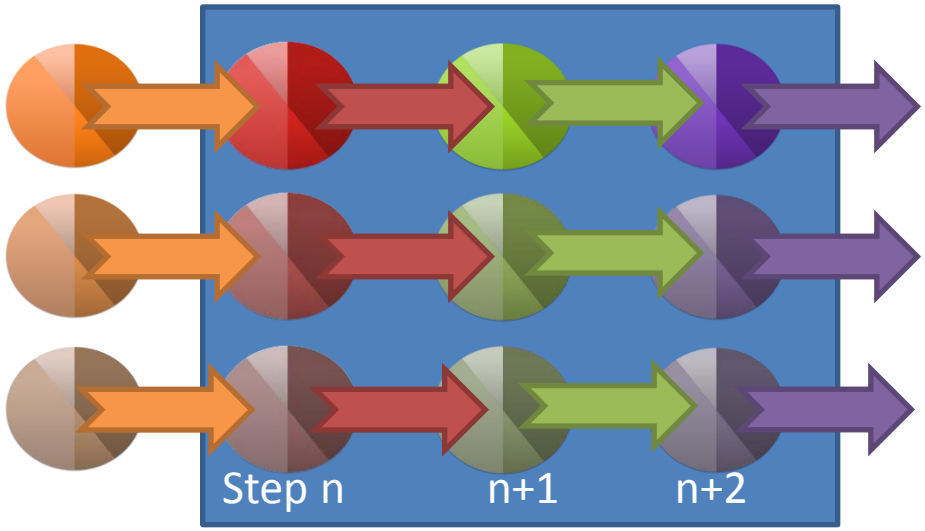
Severity of all 9 scenarios

COMBINATORICS
via FMECAENGINE automation



The perturbation is applied only to **step *n*** and then propagated to dependent steps *(e.g. local change of temperature/time)*

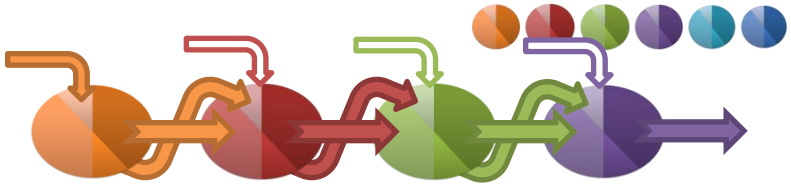
The perturbation is applied to **all steps** n,n+1,n+2,n+3…
(e.g. small/medium/large molecules)



ADVANCED EXAMPLE

INPUT TABLE (automation columns: Foscale, Kscale)

All valid Matlab syntaxes are eligible



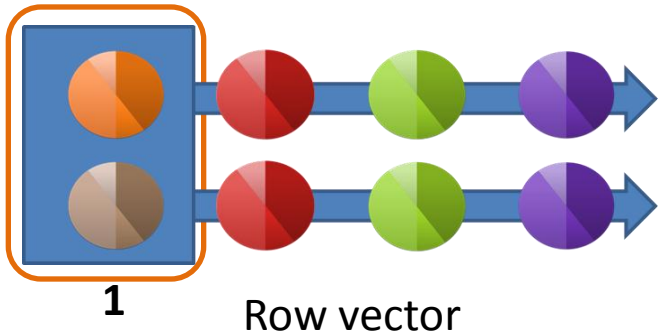
SAFEFOODPACK DESIGN

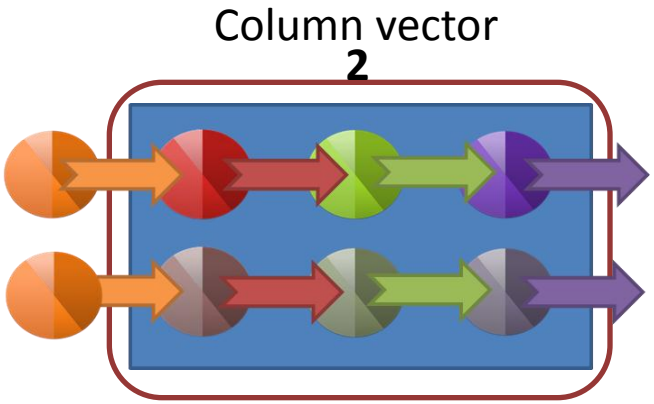
FAILURE MODE, EFFECTS, AND CRITICALITY ANALYSIS (FMECA)

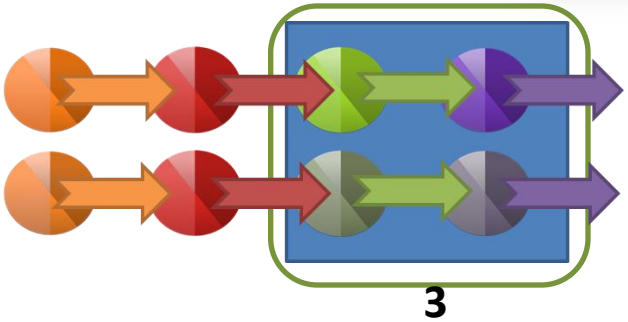
Engine="**fmecaengine**" (version **0.41**) Host="**olivier@mol10.agroparistech.fr**" (mlm release **R2010b**) Local Path="**/home/olivier/MaiNguyen/ANR_SFPD/WP2_FMECA/presentation_Mai**"
Worksheet="**sim**" Input File="**combinations_complex.ods**" FMECA Database="**fmecabaseofconditions.mat**" Input Folder="**inputs**" Output Folder="**combinations_complex**"
result page » dependence graph (pdf)

COMBINATIONS_COMPLEX.ODS | 19-MAY-2011 14:01:47 | 16.1
KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SFPD/WP2_FMECA/PRESENTATION_MAI/INPUTS

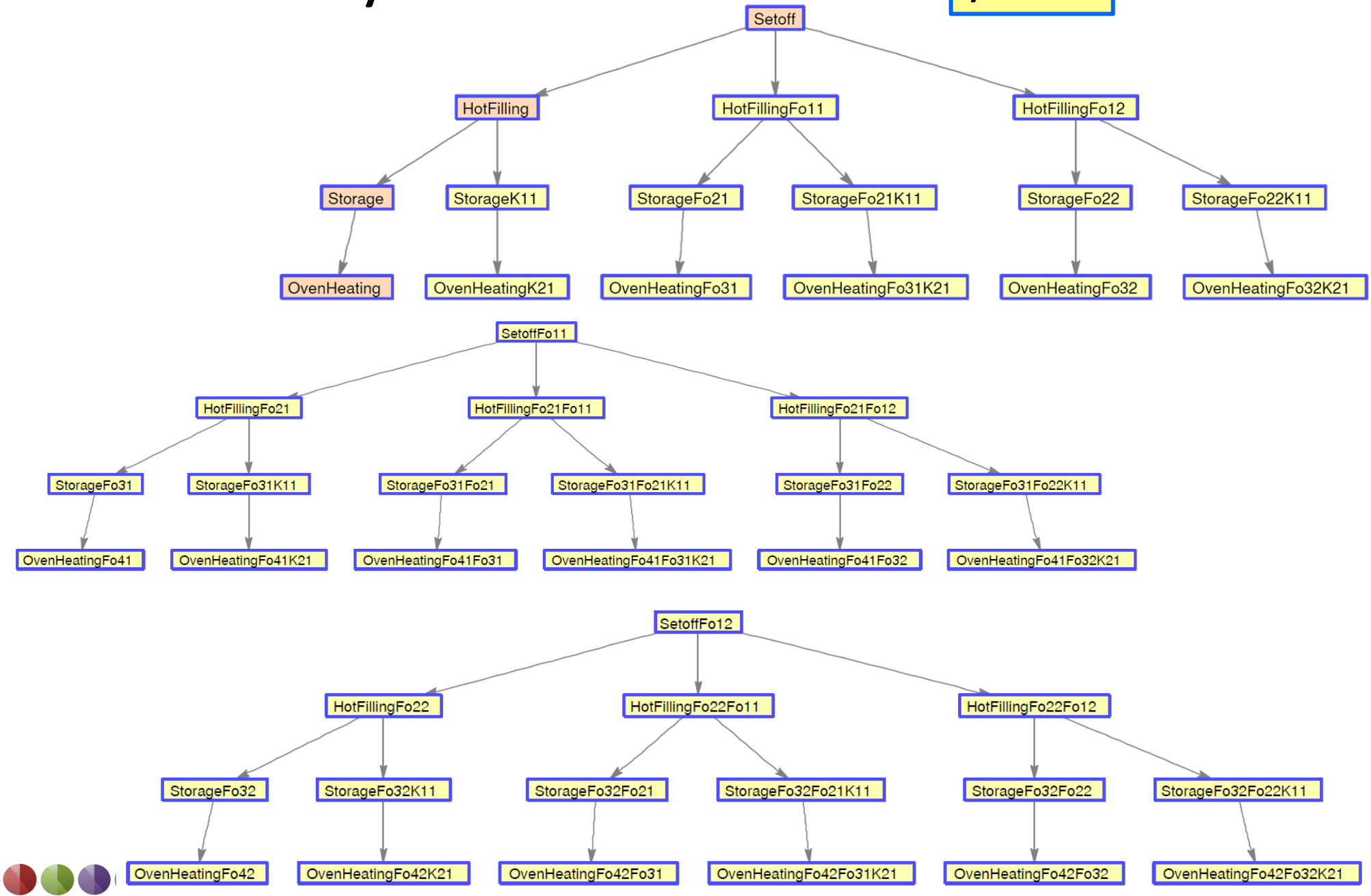
row	id	parent	Foscale	Kscale	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	*usercode*		*Foscale*	*Kscale*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
1	Setoff		[0.1 10]		8.64e+06	0.0115385	0.001	5e-05	0.0006	0	0.5	-1000	3.3e-14	1.2e-16	10	1
2	HotFilling	Setoff	[2 3]		600							1000	1.77e-11	2e-13		
3	Migration	HotFilling		[1;0.01]	1.728e+07								3.3e-14	1.2e-16		
4	OvenHeating	Migration			300								1.1e-10	3e-12		
INPUT TABLE	4 simulation definitions				date	19-May-2011 14:02:06										







Automatically created nodes are yellow



COMBINATORICS: automatic inheritance

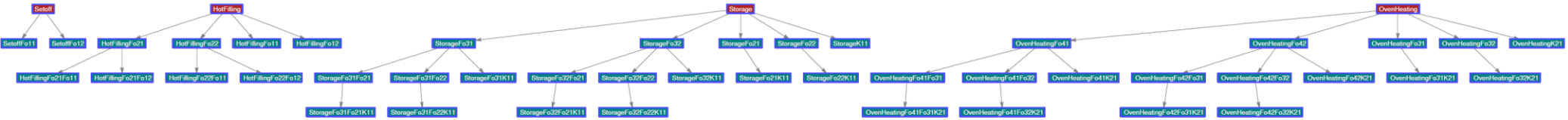


ILLUSTRATION2_FMECAENGINE.ODS | 28-AVR.-2011 22:05:39 | 14.8 KBYTES | C:\DATA\OLIVIER\INRA\ETUDIANTS & VISITEURS\AUDREY GOUJON\ILLUSTRATION_FMECA\INPUTS

nfo	inherit	row	id	parent
nfo	*inherit*	*row*	*usercode*	

nfo	inherit	row	id	parent
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Setoff.Foscale=1	StorageFo31	3	StorageFo31Fo22	HotFillingFo21Fo12
Setoff.Foscale=1	OvenHeatingFo41	4	OvenHeatingFo41Fo32	StorageFo31Fo22
Setoff.Foscale=1	HotFillingFo22	2	HotFillingFo22Fo11	SetoffFo12
Setoff.Foscale=1	StorageFo32	3	StorageFo32Fo21	HotFillingFo22Fo11
Setoff.Foscale=1	OvenHeatingFo42	4	OvenHeatingFo42Fo31	StorageFo32Fo21
Setoff.Foscale=1	HotFillingFo22	2	HotFillingFo22Fo12	SetoffFo12
Setoff.Foscale=1	StorageFo32	3	StorageFo32Fo22	HotFillingFo22Fo12
Setoff.Foscale=1	OvenHeatingFo42	4	OvenHeatingFo42Fo32	StorageFo32Fo22
Storage.Kscale=[1;0.01]	Storage	3	StorageK11	HotFilling
Storage.Kscale=0.01	OvenHeating	4	OvenHeatingK21	StorageK11
Setoff.Foscale=1	StorageFo31	3	StorageFo31K11	HotFillingFo21
Setoff.Foscale=1	OvenHeatingFo41	4	OvenHeatingFo41K21	StorageFo31K11
Setoff.Foscale=1	StorageFo32	3	StorageFo32K11	HotFillingFo22
Setoff.Foscale=1	OvenHeatingFo42	4	OvenHeatingFo42K21	StorageFo32K11
HotFilling.Foscale=2	StorageFo21	3	StorageFo21K11	HotFillingFo11
HotFilling.Foscale=2	OvenHeatingFo31	4	OvenHeatingFo31K21	StorageFo21K11
HotFilling.Foscale=3	StorageFo22	3	StorageFo22K11	HotFillingFo12
HotFilling.Foscale=3	OvenHeatingFo32	4	OvenHeatingFo32K21	StorageFo22K11
Setoff.Foscale=1	StorageFo32Fo21	3	StorageFo32Fo21K11	HotFillingFo22Fo11
		4	OvenHeatingFo42Fo31K21	StorageFo32Fo21K11
		3	StorageFo32Fo22K11	HotFillingFo22Fo12
		4	OvenHeatingFo42Fo32K21	StorageFo32Fo22K11

parent	t	I_F	I_1	I_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2	PDF	PNG	MAT	MAT
	s	m	m	m	kg/m³	kg/m³	kg/m³	no unit	m²/s	m²/s	(kg/m³)/(kg/m³)	(kg/m³)/(kg/m³)	output	output	date	size
	8.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-014	1.2e-016	10	1	document	image	30-avr.-2011 19:47:13	2.0 MBytes
	600	0.0115385	0.001	5e-005	0	0	0.5	1000	1.77e-011	2e-013	10	1	document	image	30-avr.-2011 19:47:15	1.9 MBytes
	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	10	1	document	image	30-avr.-2011 19:47:17	2.2 MBytes
	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	10	1	document	image	30-avr.-2011 19:47:19	2.0 MBytes
	0.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-015	1.2e-017	10	1	document	image	30-avr.-2011 19:47:44	2.0 MBytes
Fo11	600	0.0115385	0.001	5e-005	0	0	0.5	1000	1.77e-011	2e-013	10	1	document	image	30-avr.-2011 19:47:46	2.2 MBytes
ngFo21	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	10	1	document	image	30-avr.-2011 19:47:48	2.2 MBytes
eFo31	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	10	1	document	image	30-avr.-2011 19:47:50	2.0 MBytes
	0.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-013	1.2e-015	10	1	document	image	30-avr.-2011 19:48:16	1.6 MBytes
Fo12	600	0.0115385	0.001	5e-005	0	0	0.5	1000	1.77e-011	2e-013	10	1	document	image	30-avr.-2011 19:48:18	1.6 MBytes
ngFo22	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	10	1	document	image	30-avr.-2011 19:48:20	2.1 MBytes
eFo32	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	10	1	document	image	30-avr.-2011 19:48:22	2.0 MBytes
	600	0.0115385	0.001	5e-005	0	0	0.5	1000	3.54e-011	4e-013	10	1	document	image	30-avr.-2011 19:47:25	2.0 MBytes
ngFo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	10	1	document	image	30-avr.-2011 19:47:27	2.2 MBytes
eFo21	300	0.0115385	0.001	5e-005	0	0	0.5	1000	2.2e-010	6e-012	10	1	document	image	30-avr.-2011 19:47:29	2.0 MBytes
	600	0.0115385	0.001	5e-005	0	0	0.5	1000	5.31e-011	6e-013	10	1	document	image	30-avr.-2011 19:47:35	2.0 MBytes
ngFo12	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	9.9e-014	3.6e-016	10	1	document	image	30-avr.-2011 19:47:37	2.2 MBytes
eFo22	300	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-010	9e-012	10	1	document	image	30-avr.-2011 19:47:39	2.0 MBytes
Fo11	600	0.0115385	0.001	5e-005	0	0	0.5	1000	3.54e-011	4e-013	10	1	document	image	30-avr.-2011 19:47:56	2.2 MBytes
ngFo21Fo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	10	1	document	image	30-avr.-2011 19:47:58	2.2 MBytes
eFo31Fo21	300	0.0115385	0.001	5e-005	0	0	0.5	1000	2.2e-010	6e-012	10	1	document	image	30-avr.-2011 19:48:00	2.0 MBytes
Fo11	600	0.0115385	0.001	5e-005	0	0	0.5	1000	5.31e-011	6e-013	10	1	document	image	30-avr.-2011 19:48:06	2.2 MBytes
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Fo12	600	0.0115385	0.001	5e-005	0	0	0.5	1000	3.54e-011	4e-013	10	1	document	image	30-avr.-2011 19:48:28	1.7 MBytes
ngFo22Fo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	10	1	document	image	30-avr.-2011 19:48:30	2.2 MBytes
eFo32Fo21	300	0.0115385	0.001	5e-005	0	0	0.5	1000	2.2e-010	6e-012	10	1	document	image	30-avr.-2011 19:48:32	2.0 MBytes
Fo12	600	0.0115385	0.001	5e-005	0	0	0.5	1000	5.3[illegible]	[illegible]	10	1	document	image	30-avr.-2011 19:48:38	1.8 MBytes
ngFo22Fo12	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	9.9[illegible]	[illegible]	10	1	document	image	30-avr.-2011 19:48:40	2.2 MBytes
eFo32Fo22	300	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3[illegible]	9e-012	10	1	document	image	30-avr.-2011 19:48:42	2.0 MBytes
ng	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	0.1	0.01	document	image	30-avr.-2011 19:47:21	2.1 MBytes
eK11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	0.1	0.01	document	image	30-avr.-2011 19:47:23	1.9 MBytes
ngFo21	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	0.1	0.01	document	image	30-avr.-2011 19:47:52	2.2 MBytes
eFo31K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	0.1	0.01	document	image	30-avr.-2011 19:47:54	2.0 MBytes
ngFo22	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-014	1.2e-016	0.1	0.01	document	image	30-avr.-2011 19:48:24	2.1 MBytes
eFo32K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	1.1e-010	3e-012	0.1	0.01	document	image	30-avr.-2011 19:48:26	1.9 MBytes
ngFo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	0.1	0.01	document	image	30-avr.-2011 19:47:31	2.2 MBytes
eFo21K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	2.2e-010	6e-012	0.1	0.01	document	image	30-avr.-2011 19:47:33	1.9 MBytes
ngFo12	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	9.9e-014	3.6e-016	0.1	0.01	document	image	30-avr.-2011 19:47:41	2.1 MBytes
eFo22K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-010	9e-012	0.1	0.01	document	image	30-avr.-2011 19:47:43	1.8 MBytes
ngFo21Fo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	0.1	0.01	document	image	30-avr.-2011 19:48:02	2.2 MBytes
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ngFo21Fo12	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	9.9e-014	3.6e-016	0.1	0.01	document	image	30-avr.-2011 19:48:12	2.2 MBytes
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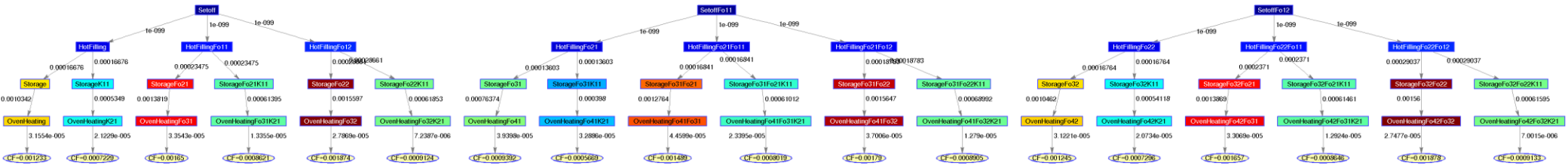
ngFo22Fo11	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	6.6e-014	2.4e-016	0.1	0.01	document	image	30-avr.-2011 19:48:34	2.1 MBytes
eFo32Fo21K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	2.2e-010	6e-012	0.1	0.01	document	image	30-avr.-2011 19:48:36	1.9 MBytes
ngFo22Fo12	1.728e+007	0.0115385	0.001	5e-005	0	0	0.5	1000	9.9e-014	3.6e-016	0.1	0.01	document	image	30-avr.-2011 19:48:44	2.1 MBytes
eFo32Fo22K11	300	0.0115385	0.001	5e-005	0	0	0.5	1000	3.3e-010	9e-012	0.1	0.01	document	image	30-avr.-2011 19:48:46	1.8 MBytes

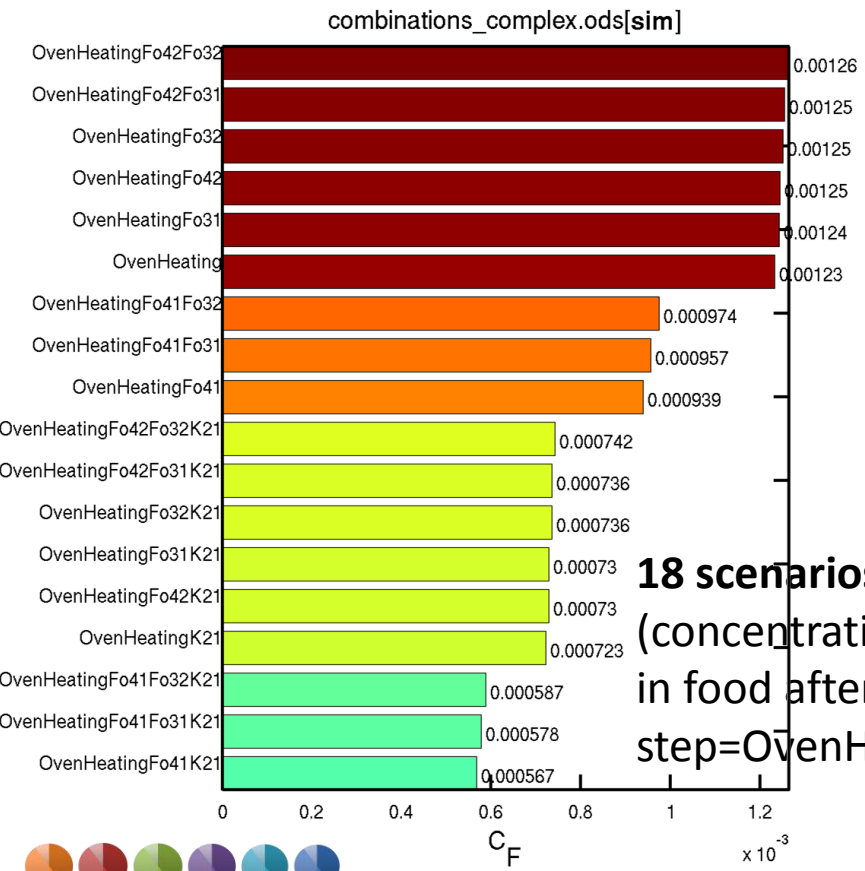
OUTPUT TABLE

FMECA database 48 simulations

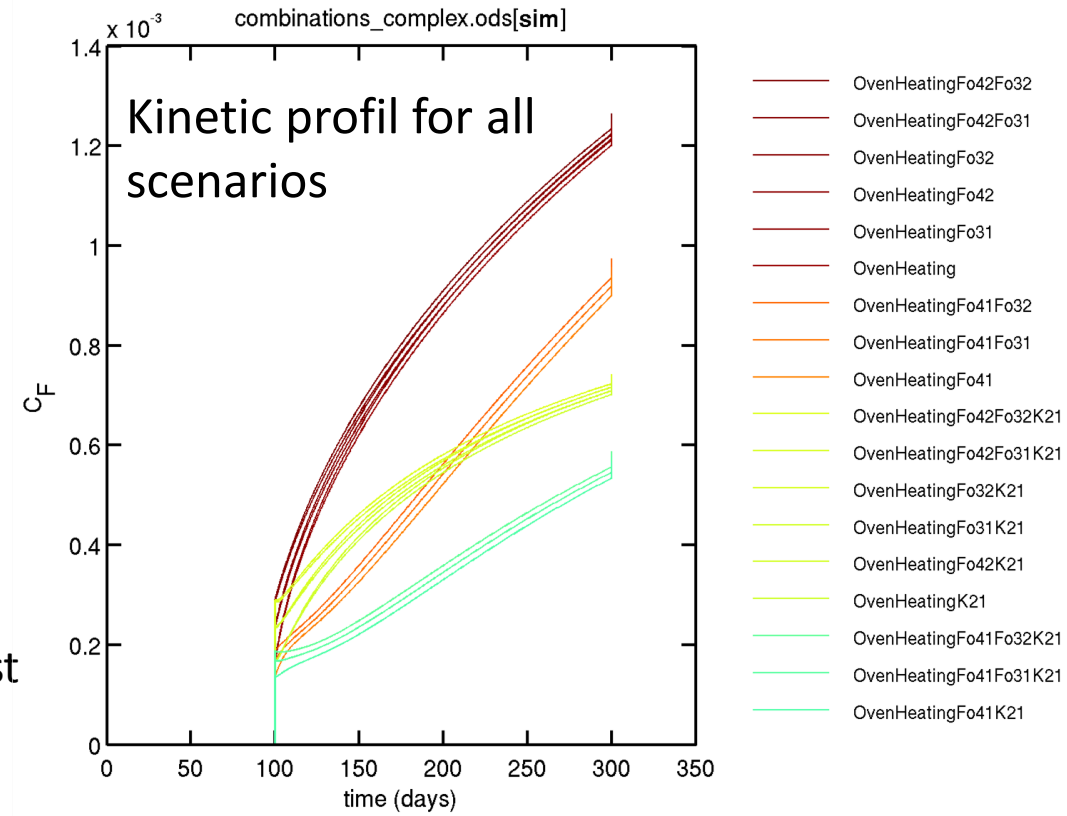
fmecabaseofconditions.mat **last update** 30-avr.-2011 21:39:17 **last report** 0 simulations updated/created in 2.047 s

ADVANCED EXAMPLE: Results





18 scenarios (concentration in food after the last step=OvenHeating)

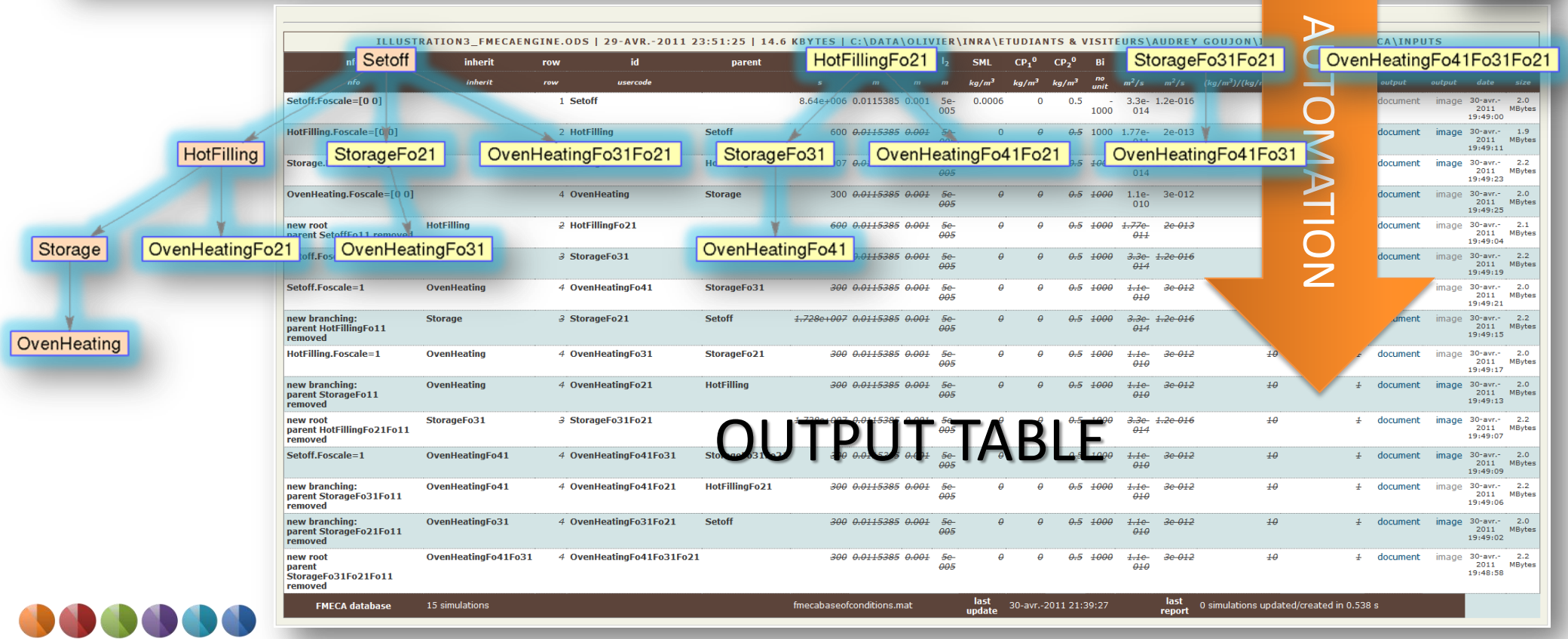


COMBINATORICS: OMITTING STEPS

ILLUSTRATION3_FMECAENGINE.ODS | 29-AVR.-2011 23:51:25 | 14.6 KBYTES | C:\DATA\OLIVIER\INRA\ETUDIANTS & VISITEURS\AUDREY GOUJON\ILLUSTRATION_FMECA\INPUTS

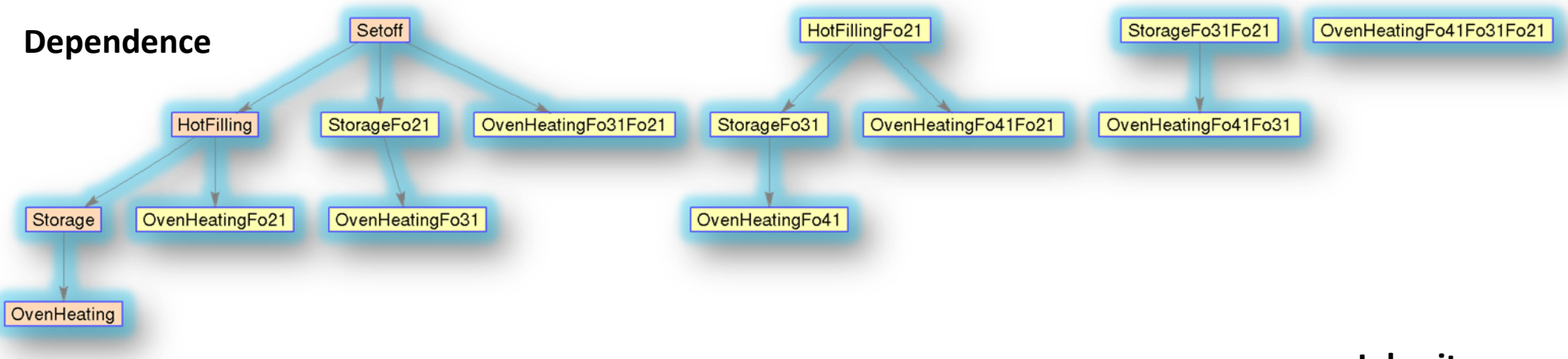
row	id	parent	Foscale	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	*usercode*		*Foscale*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
1	Setoff		[0 0]	8.64e+006	0.0115385	0.001	5e-005	0.0006	0	0.5	-1000	3.3e-014	1.2e-016	10	1
2	HotFilling	Setoff	[0 0]	600				0			1000	1.77e-011	2e-013		
3	Storage	HotFilling	[0 0]	1.728e+007				~~0~~				3.3e-014	1.2e-016		
4	OvenHeating	Storage	[0 0]	300				~~0~~				1.1e-010	3e-012		

INPUT TABLE 4 simulation definitions date 30-Apr-2011 21:39:25

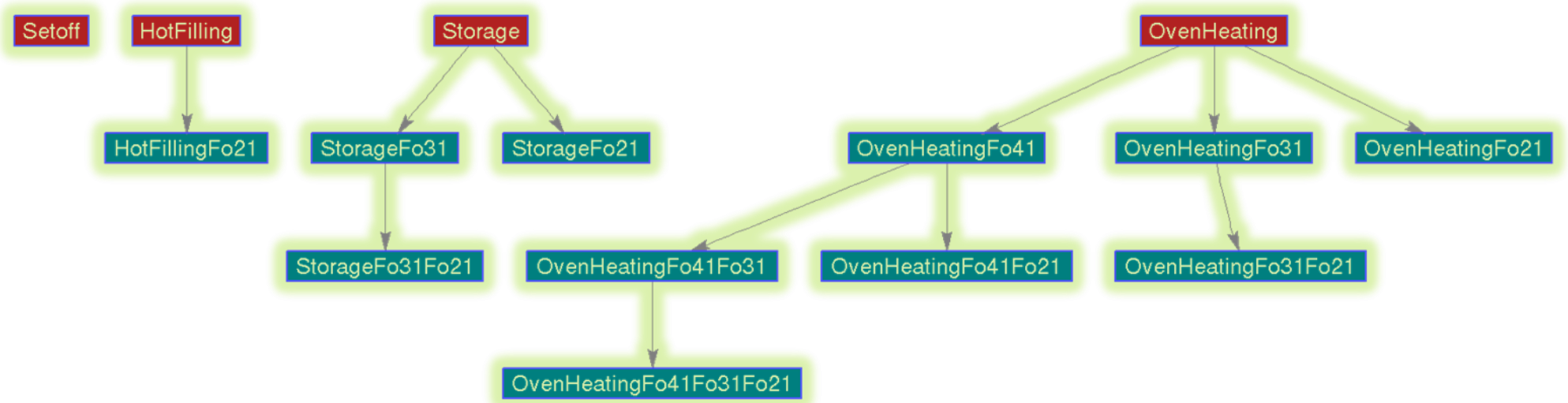


OMITTING STEPS: FMECAENGINE builds all trees required to assess the effects of all combinations

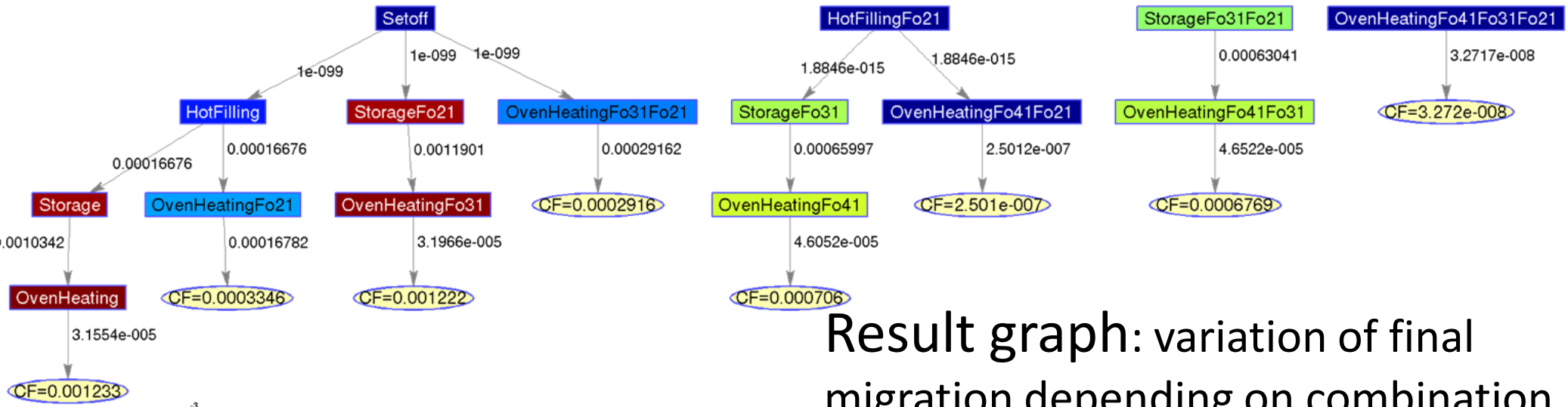
Dependence



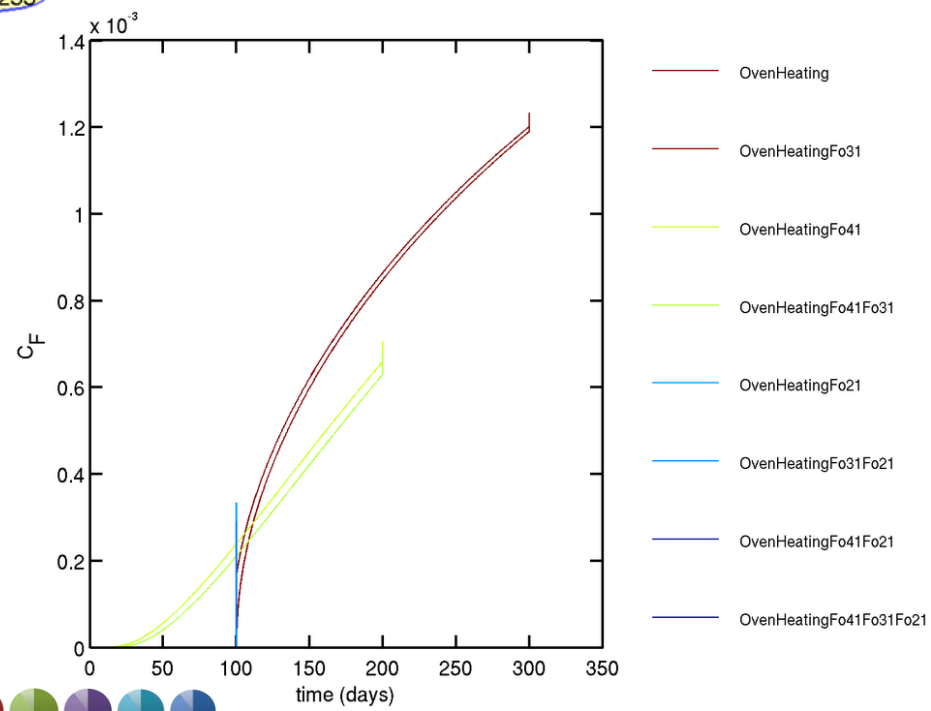
Inheritance



OMITTING STEPS: Results

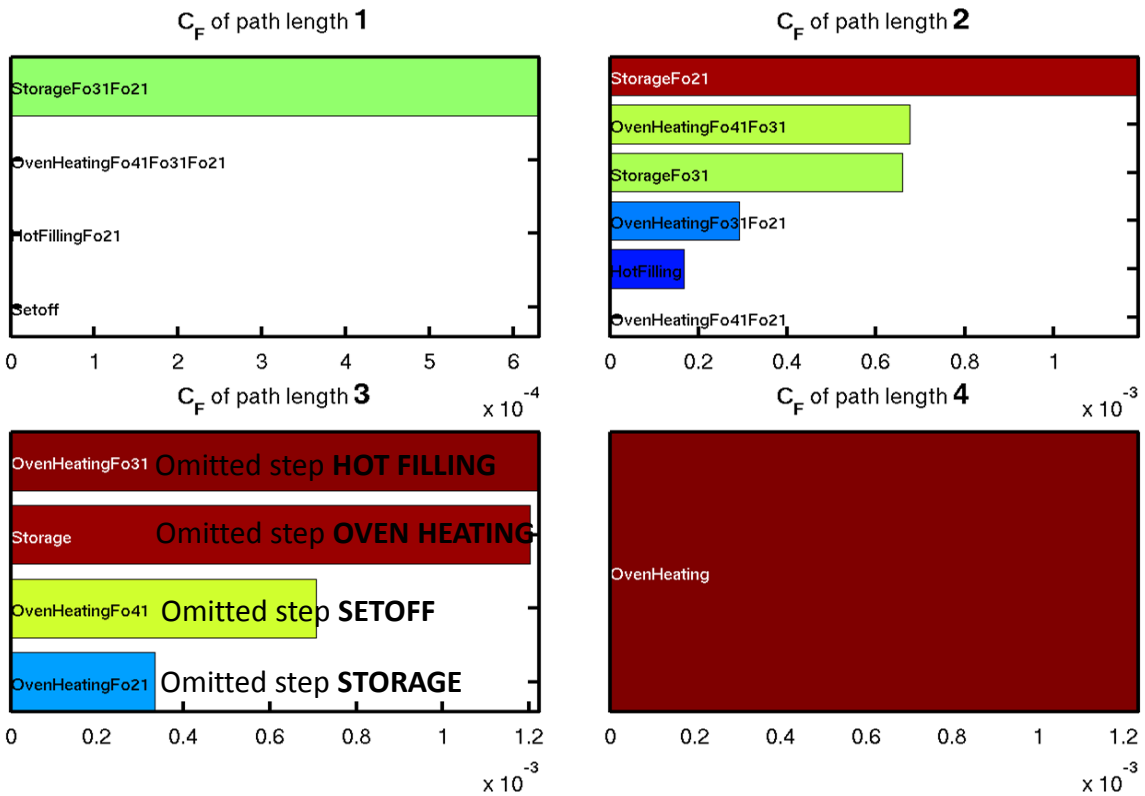


Result graph: variation of final migration depending on combination

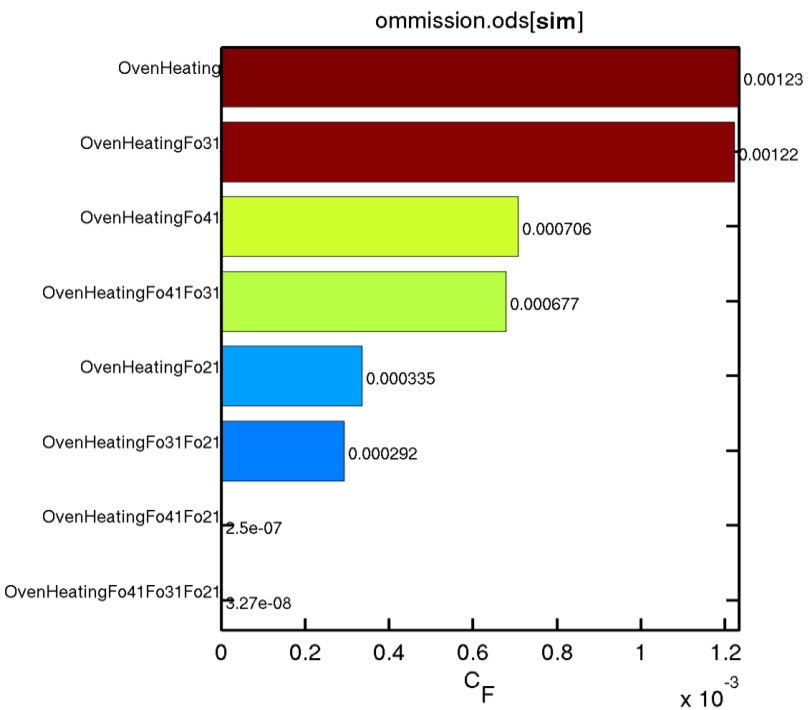


Kinetic graph: concentration profil in food for all steps (color corresponds to severity of final migration)

OMITTING STEPS: Results



Final concentration in food for each scenario length



8 scenarios

(concentration in food after the last step=OvenHeating)

COMPLEX ANALYSES WITH OMITTED STEPS

A path towards FMECA-based risk assessment

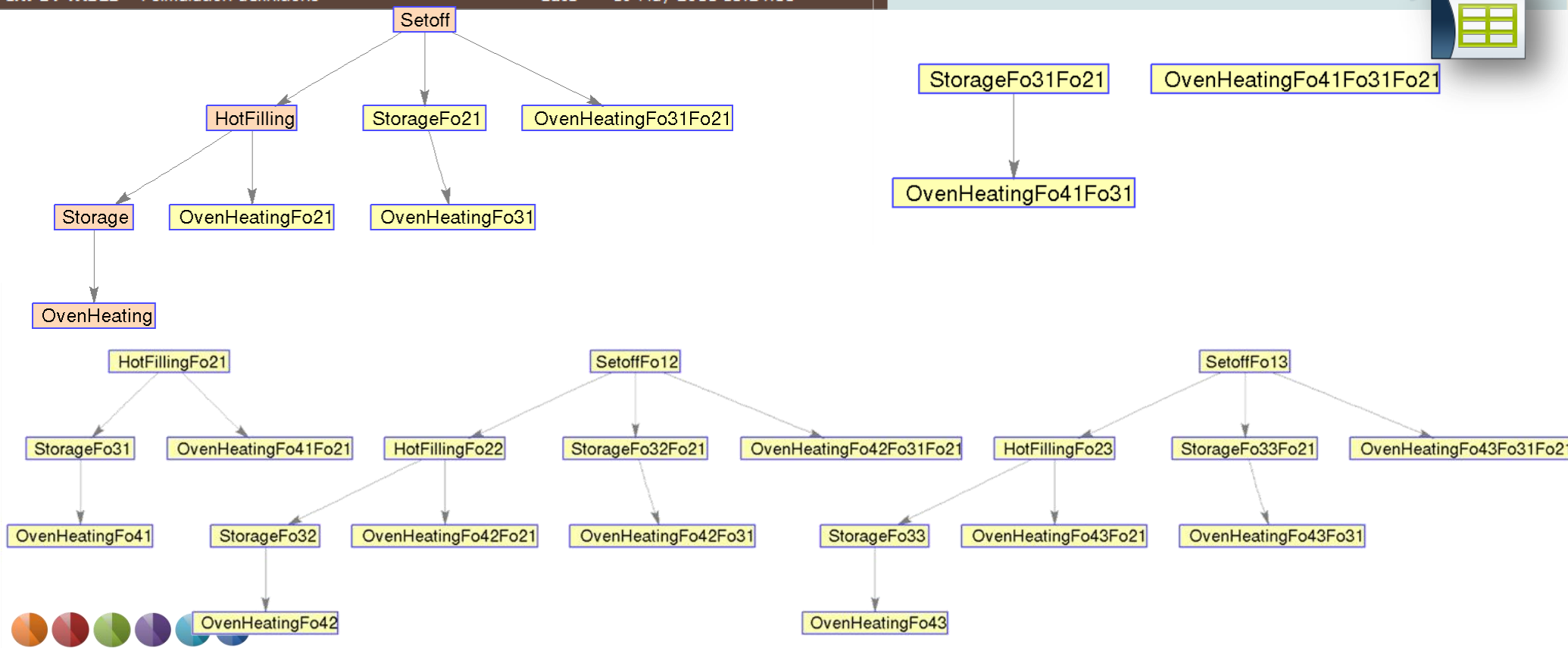
Small/large diffusants

Good/poor chemical affinity

OMISSION_COMPLEX.ODS | 19-MAY-2011 13:23:39 | 16.1
KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SFPD/WP2_FMECA/PRESENTATION_MAI/INPUTS

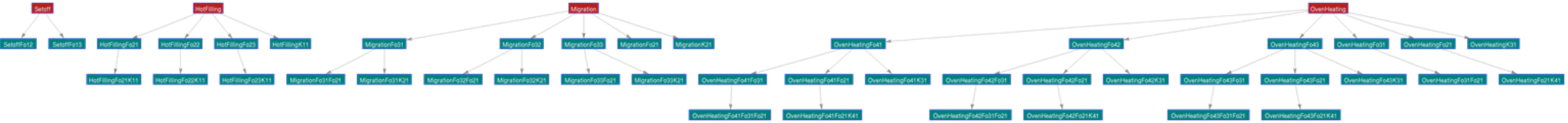
row	id	parent	Foscale	Kscale	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	usercode		Foscale	Kscale	s	m	m	m	kg/m^3	kg/m^3	kg/m^3	no unit	m^2/s	m^2/s	$(kg/m^3)/(kg/m^3)$	$(kg/m^3)/(kg/m^3)$
1	Setoff		[0 0.2 5]		8.64e+06	0.0115385	0.001	5e-05	0.0006	0	0.5	-1000	3.3e-14	1.2e-16	10	1
2	HotFilling	Setoff	[0 0]	[1;0.01]	600							1000	1.77e-11	2e-13		
3	Migration	HotFilling	[0 0]		1.728e+07								3.3e-14	1.2e-16		
4	OvenHeating	Migration	[0 0]		300								1.1e-10	3e-12		

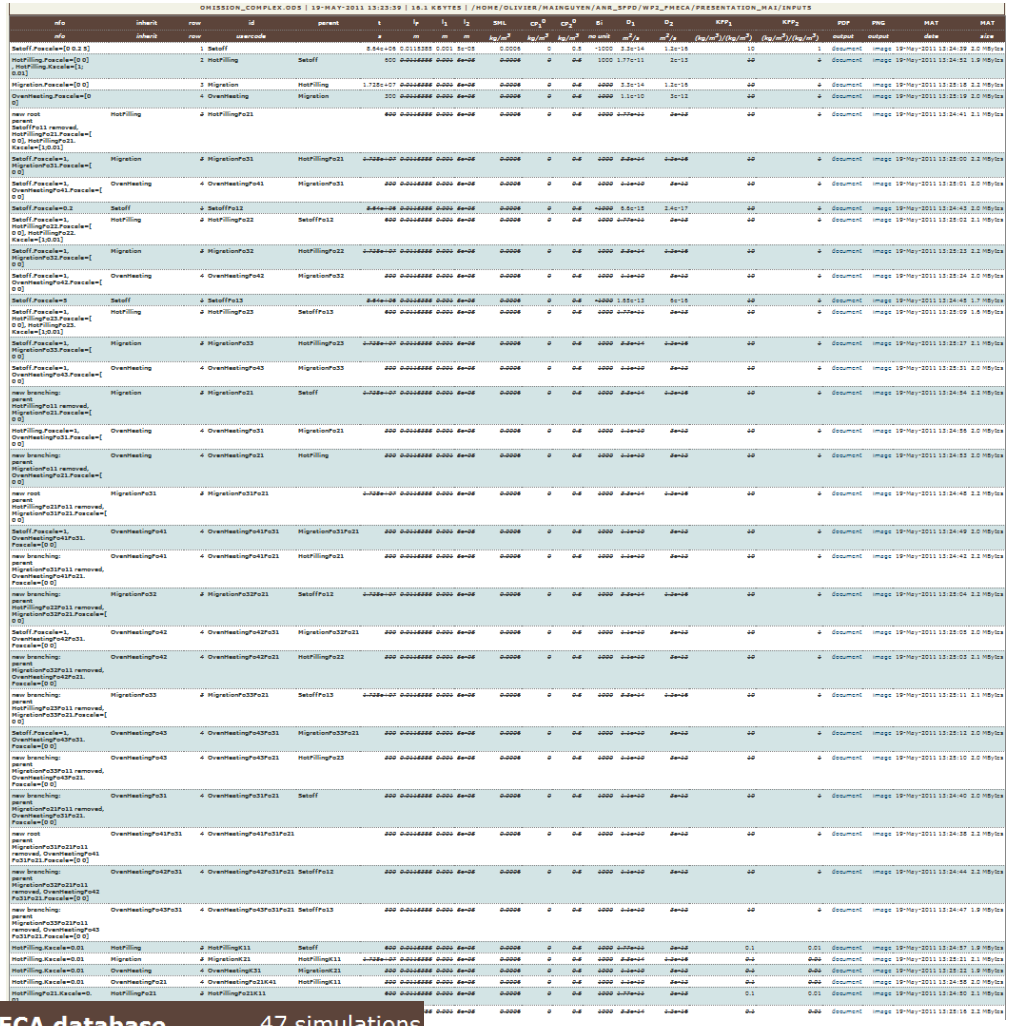
INPUT TABLE 4 simulation definitions date 19-May-2011 13:24:33



COMPLEX ANALYSES WITH OMITTED STEPS

A path towards FMECA



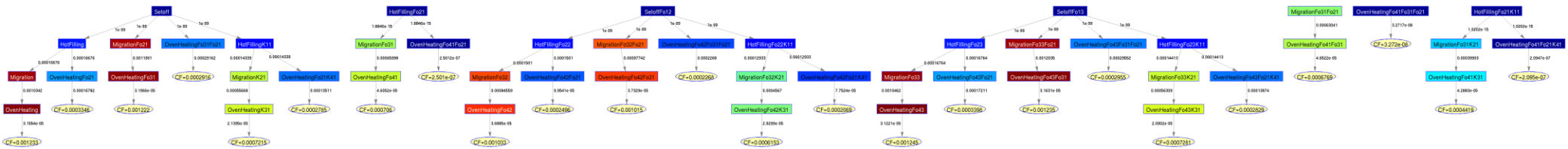


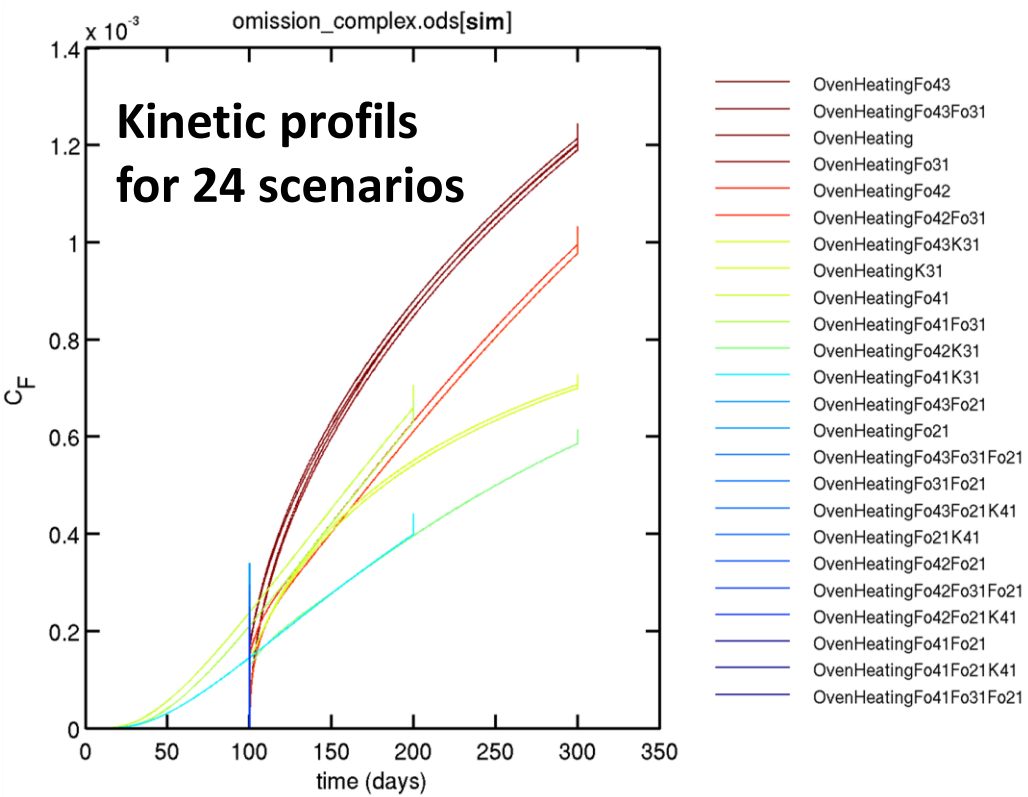
OMISSION_COMPLEX.DOS | 19-MAY-2011 13:23:39 | 16.1 KBYTES | /HOME/OLIVIER/MAINGUYEN/ANR_SPPD/WP2_FMECA/PRESENTATION_MAI/INPUTS

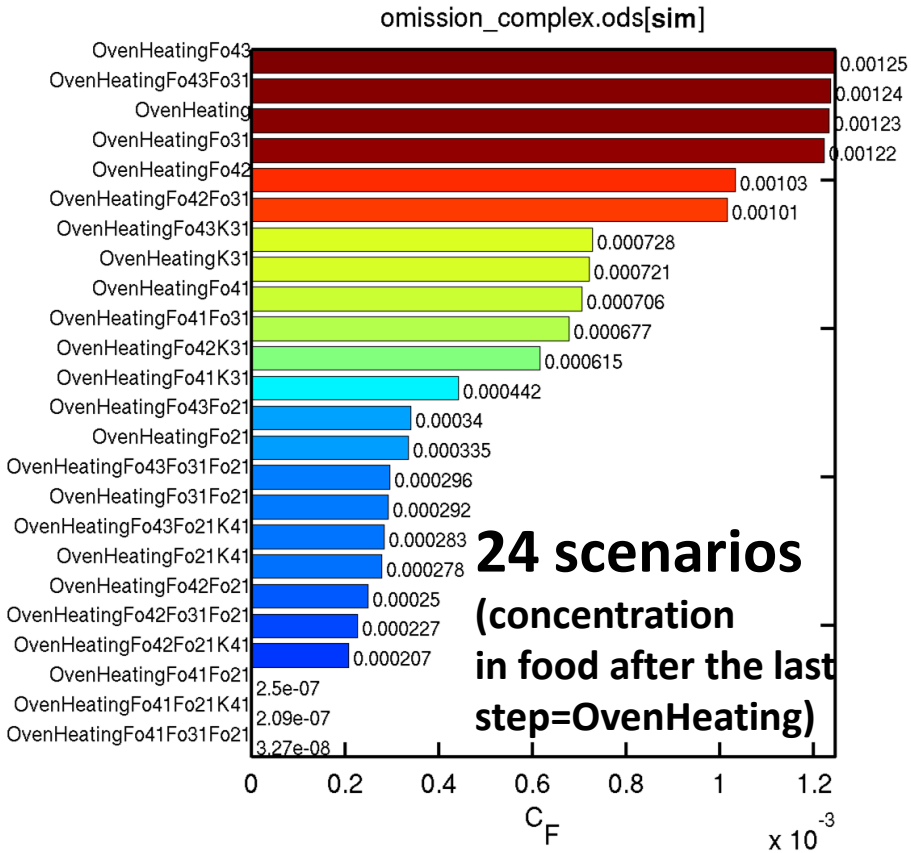
info	inherit	row	id	parent	t	t_r	t_1	t_2	SML	CF_1^0	CF_2^0	Ei	D_1	D_2	KFP_1	KFP_2	PDF	PNG	MAT	MAT
info	inherit	row	usercode		s	m			kg/m^3	kg/m^3	kg/m^3	no unit	m^2/s	m^2/s	$(kg/m^3)/(kg/m^3)$	$(kg/m^3)/(kg/m^3)$	output	output	date	size
Setoff.Foscale=[0 0.2 0]		1	Setoff		8.64e+05	0.015385	0.001	6e-05	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	1	document	image	19-May-2011 13:24:39	2.0 Mb/ks
HotFilling.Foscale=[0 0] , HotFilling.Kscale=[1; 0.01]		2	HotFilling	Setoff	500	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.77e-11	2e-13	10	4	document	image	19-May-2011 13:24:52	1.9 Mb/ks
Migration.Foscale=[0 0]		3	Migration	HotFilling	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:18	2.2 Mb/ks
OvenHeating.Foscale=[0 0]		4	OvenHeating	Migration	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:19	2.0 Mb/ks
new root parent SetoffFo11 removed, HotFillingFo21.Foscale=[0 0], HotFillingFo21. Kscale=[1;0.01]	HotFilling	4	HotFillingFo21		600	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1e-16	10	4	document	image	19-May-2011 13:24:41	2.1 Mb/ks
Setoff.Foscale=1, MigrationFo31.Foscale=[0 0]	Migration	4	MigrationFo31	HotFillingFo21	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:00	2.2 Mb/ks
Setoff.Foscale=1, OvenHeatingFo41.Foscale=[0 0]	OvenHeating	4	OvenHeatingFo41	MigrationFo31	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:01	2.0 Mb/ks
Setoff.Foscale=0.2	Setoff	4	SetoffFo12		8.64e+06	0.016666	0.001	6e-06	0.0006	0	0.8	10000	5.5e-13	2.4e-17	10	4	document	image	19-May-2011 13:24:43	2.0 Mb/ks
Setoff.Foscale=1, HotFillingFo22.Foscale=[0 0], HotFillingFo22. Kscale=[1;0.01]	HotFilling	4	HotFillingFo22	SetoffFo12	600	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1e-16	10	4	document	image	19-May-2011 13:25:02	2.1 Mb/ks
Setoff.Foscale=1, MigrationFo32.Foscale=[0 0]	Migration	4	MigrationFo32	HotFillingFo22	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:23	2.2 Mb/ks
Setoff.Foscale=1, OvenHeatingFo42.Foscale=[0 0]	OvenHeating	4	OvenHeatingFo42	MigrationFo32	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:24	2.0 Mb/ks
Setoff.Foscale=5	Setoff	4	SetoffFo13		8.64e+06	0.016666	0.001	6e-06	0.0006	0	0.8	10000	1.55e-13	6e-18	10	4	document	image	19-May-2011 13:24:45	1.7 Mb/ks
Setoff.Foscale=1, HotFillingFo23.Foscale=[0 0], HotFillingFo23. Kscale=[1;0.01]	HotFilling	4	HotFillingFo23	SetoffFo13	600	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1e-16	10	4	document	image	19-May-2011 13:25:09	1.6 Mb/ks
Setoff.Foscale=1, MigrationFo33.Foscale=[0 0]	Migration	4	MigrationFo33	HotFillingFo23	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:27	2.1 Mb/ks
Setoff.Foscale=1, OvenHeatingFo43.Foscale=[0 0]	OvenHeating	4	OvenHeatingFo43	MigrationFo33	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:31	2.0 Mb/ks
new branching: parent HotFillingFo11 removed, MigrationFo21.Foscale=[0 0]	Migration	4	MigrationFo21	Setoff	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:24:54	2.2 Mb/ks
HotFilling.Foscale=1, OvenHeatingFo31.Foscale=[0 0]	OvenHeating	4	OvenHeatingFo31	MigrationFo21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:55	2.0 Mb/ks
new branching: parent MigrationFo11 removed, OvenHeatingFo21.Foscale=[0 0]	OvenHeating	4	OvenHeatingFo21	HotFilling	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:53	2.0 Mb/ks
new root parent HotFillingFo21Fo11 removed, MigrationFo31Fo21.Foscale=[0 0]	MigrationFo31	4	MigrationFo31Fo21		1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:24:48	2.2 Mb/ks
Setoff.Foscale=1, OvenHeatingFo41.Foscale=[0 0]	OvenHeatingFo41	4	OvenHeatingFo41Fo31	MigrationFo31Fo21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:49	2.0 Mb/ks
new branching: parent MigrationFo31Fo11 removed, OvenHeatingFo41Fo21. Foscale=[0 0]	OvenHeatingFo41	4	OvenHeatingFo41Fo21	HotFillingFo21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:42	2.2 Mb/ks
new branching: parent HotFillingFo22Fo11 removed, MigrationFo32Fo21.Foscale=[0 0]	MigrationFo32	4	MigrationFo32Fo21	SetoffFo12	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:04	2.2 Mb/ks
Setoff.Foscale=1, OvenHeatingFo42.Foscale=[0 0]	OvenHeatingFo42	4	OvenHeatingFo42Fo31	MigrationFo32Fo21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:05	2.0 Mb/ks
new branching: parent MigrationFo32Fo11 removed, OvenHeatingFo42Fo21. Foscale=[0 0]	OvenHeatingFo42	4	OvenHeatingFo42Fo21	HotFillingFo22	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:03	2.1 Mb/ks
new branching: parent HotFillingFo23Fo11 removed, MigrationFo33Fo21.Foscale=[0 0]	MigrationFo33	4	MigrationFo33Fo21	SetoffFo13	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	10	4	document	image	19-May-2011 13:25:11	2.1 Mb/ks
Setoff.Foscale=1, OvenHeatingFo43Fo31. Foscale=[0 0]	OvenHeatingFo43	4	OvenHeatingFo43Fo31	MigrationFo33Fo21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:12	2.0 Mb/ks
new branching: parent MigrationFo33Fo11 removed, OvenHeatingFo43Fo21. Foscale=[0 0]	OvenHeatingFo43	4	OvenHeatingFo43Fo21	HotFillingFo23	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:25:10	2.0 Mb/ks
new branching: parent MigrationFo21Fo11 removed, OvenHeatingFo31Fo21. Foscale=[0 0]	OvenHeatingFo31	4	OvenHeatingFo31Fo21	Setoff	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:40	2.0 Mb/ks
new root parent MigrationFo31Fo21Fo11 removed, OvenHeatingFo41 Fo31Fo21.Foscale=[0 0]	OvenHeatingFo41Fo31	4	OvenHeatingFo41Fo31Fo21		300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:38	2.2 Mb/ks
new branching: parent MigrationFo32Fo21Fo11 removed, OvenHeatingFo42 Fo31Fo21.Foscale=[0 0]	OvenHeatingFo42Fo31	4	OvenHeatingFo42Fo31Fo21	SetoffFo12	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:44	2.2 Mb/ks
new branching: parent MigrationFo33Fo21Fo11 removed, OvenHeatingFo43 Fo31Fo21.Foscale=[0 0]	OvenHeatingFo43Fo31	4	OvenHeatingFo43Fo31Fo21	SetoffFo13	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	10	4	document	image	19-May-2011 13:24:47	1.9 Mb/ks
HotFilling.Kscale=0.01	HotFilling	4	HotFillingK11	Setoff	600	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1e-16	0.1	0.01	document	image	19-May-2011 13:24:57	1.9 Mb/ks
HotFilling.Kscale=0.01	Migration	4	MigrationK21	HotFillingK11	1.728e+07	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1.2e-16	0.1	0.01	document	image	19-May-2011 13:25:21	2.1 Mb/ks
HotFilling.Kscale=0.01	OvenHeating	4	OvenHeatingK31	MigrationK21	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	0.1	0.01	document	image	19-May-2011 13:25:22	1.9 Mb/ks
HotFilling.Kscale=0.01	OvenHeatingFo21	4	OvenHeatingFo21K41	HotFillingK11	300	0.016666	0.001	6e-06	0.0006	0	0.8	1000	1.1e-10	3e-12	0.1	0.01	document	image	19-May-2011 13:24:55	2.0 Mb/ks
HotFillingFo21.Kscale=0. 01	HotFillingFo21	4	HotFillingFo21K11		600	0.016666	0.001	6e-06	0.0006	0	0.8	1000	3.3e-14	1e-16	0.1	0.01	document	image	19-May-2011 13:24:50	2.1 Mb/ks
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	document	image	19-May-2011 13:25:16	2.2 Mb/ks

FMECA database 47 simulations

COMPLEX ANALYSES WITH OMITTED STEPS: Results





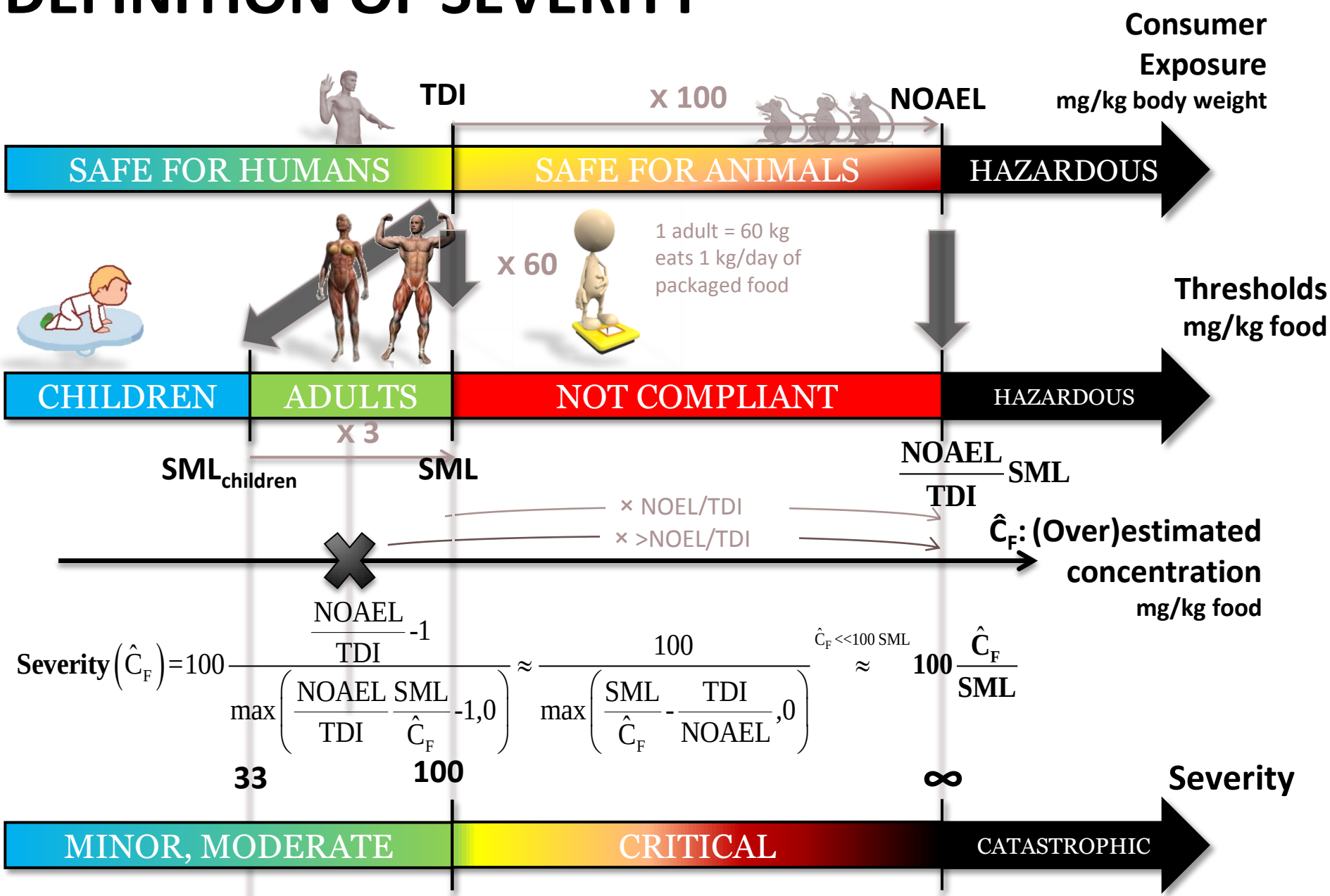


SEVERITY AND CRITICALITY ANALYSIS

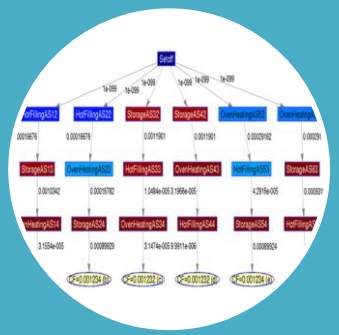
Definition of severity

3 rules for risk migration and management → illustrative example

DEFINITION OF SEVERITY

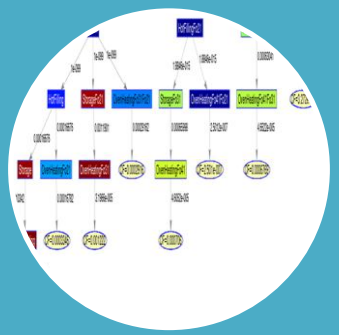


THE SELECTED EXAMPLE ILLUSTRATES NON-INTUITIVE **GROUND RULES** FOR RISK MITIGATION AND MANAGEMENT



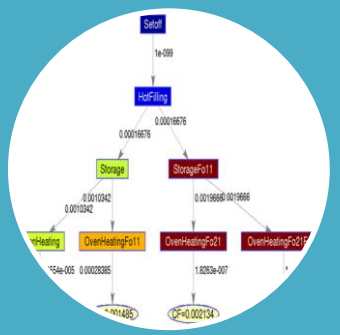
RULE 1

The final migration (consequence) in food does not depend on the order of « contamination » steps.



RULE 2

As migration is cumulative, the individual contribution of each step depends on its position in flowchart. An assessment of modal criticality independent of position is obtained by assessing the final migration without the step to evaluate.

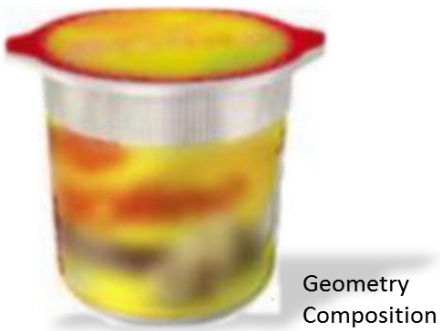


RULE 3

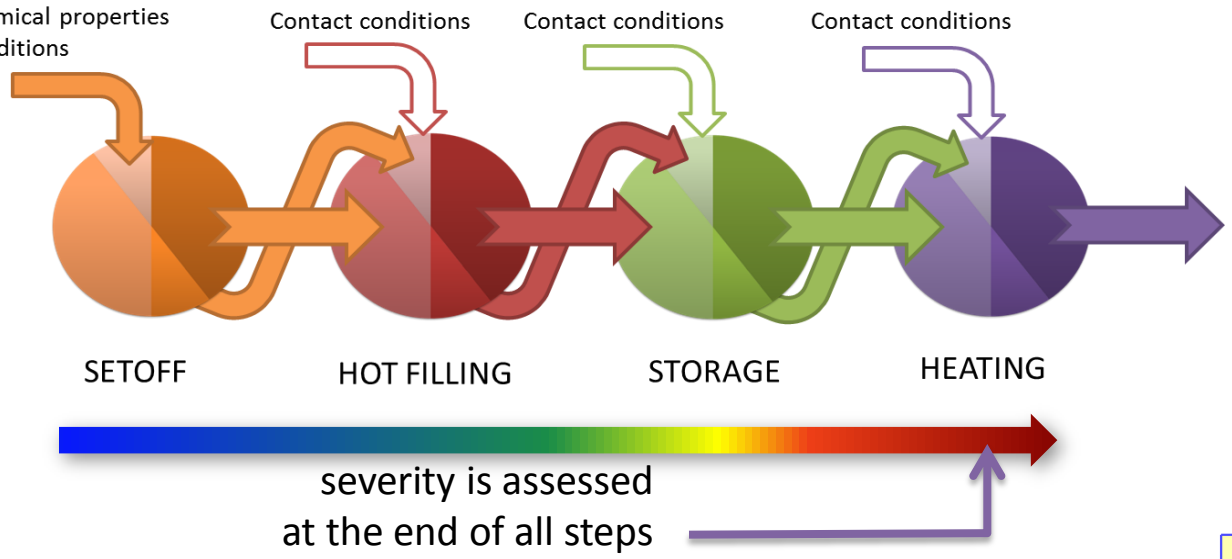
The effect of conditional probabilities must be assessed on the final migration.

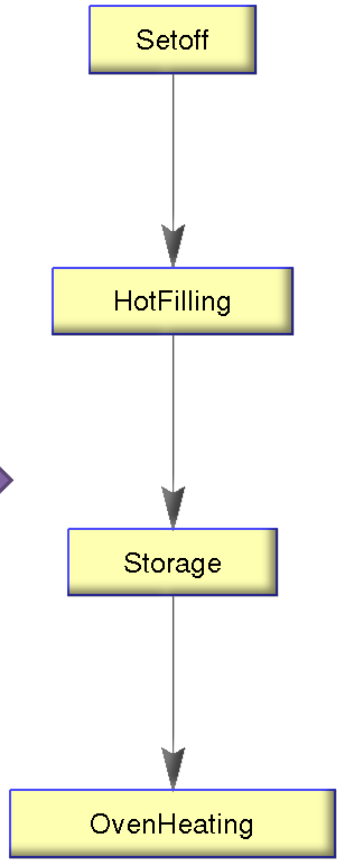
IMPLEMENTED GROUND RULES

CASE STUDY



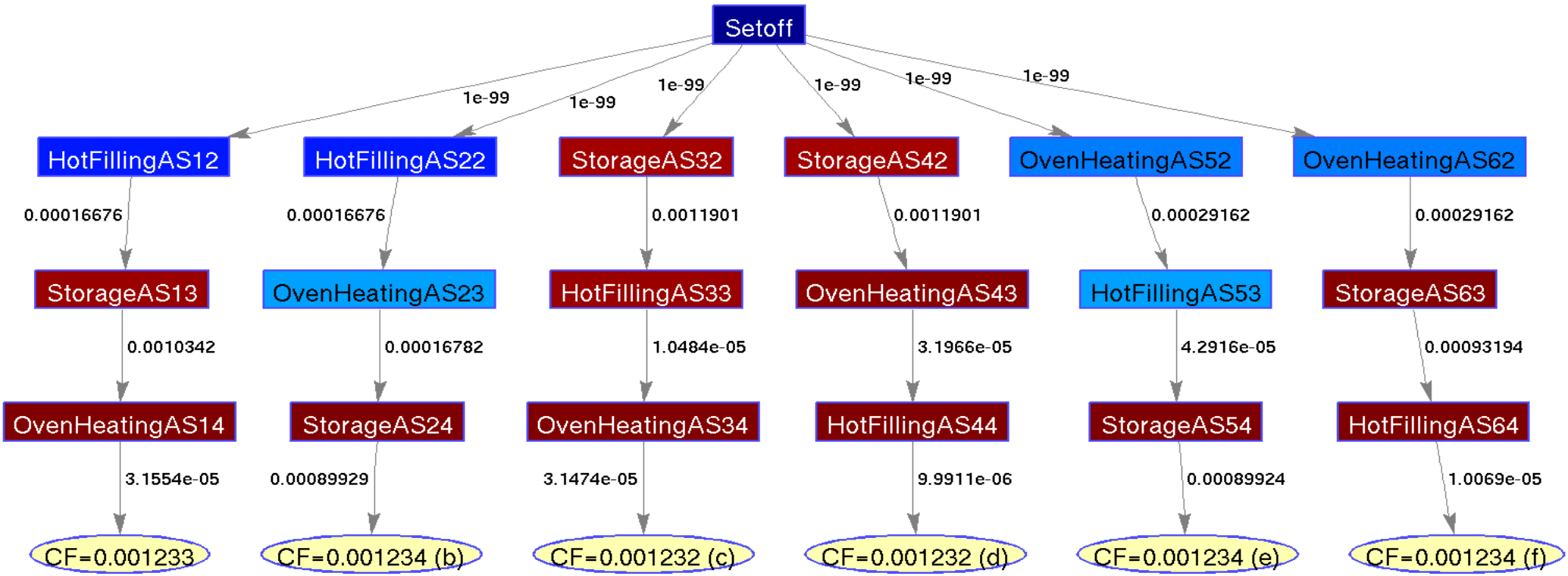
Geometry
Composition
Physico-chemical properties
Contact conditions





RISK PRIORITIZATION WITH **FMECAENGINE**

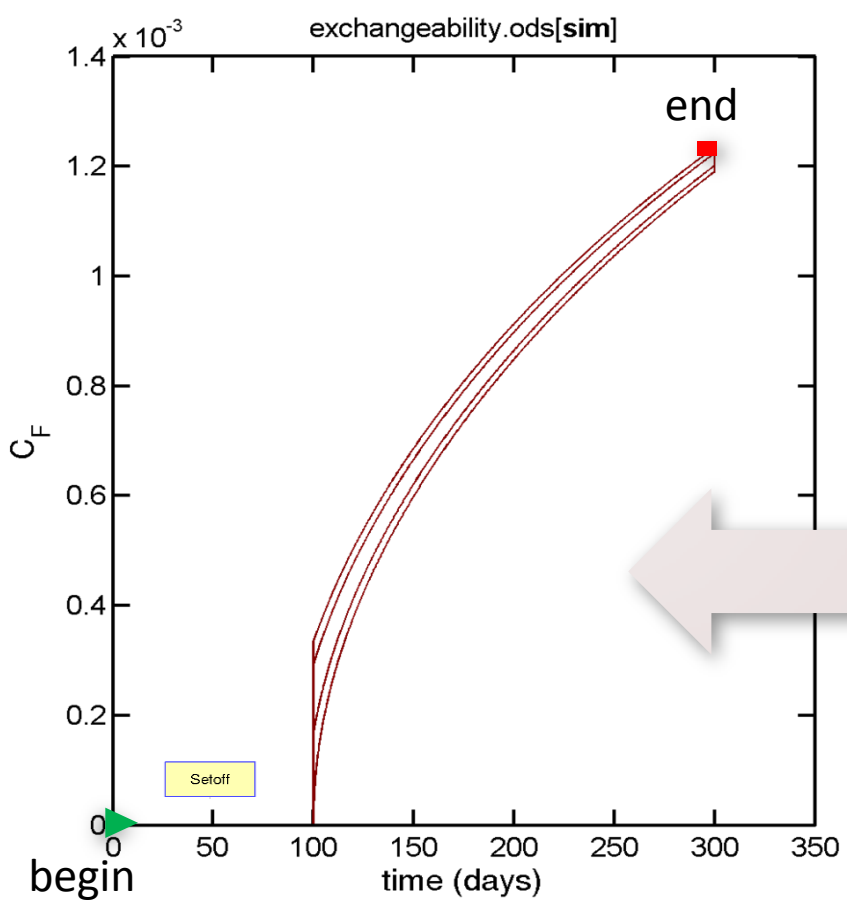
RULE 1: PERMUTING STEPS (involving a contact with food) DOES NOT CHANGE THE FINAL MIGRATION



EXCHANGEABILITY : SAME $\hat{C}_F$

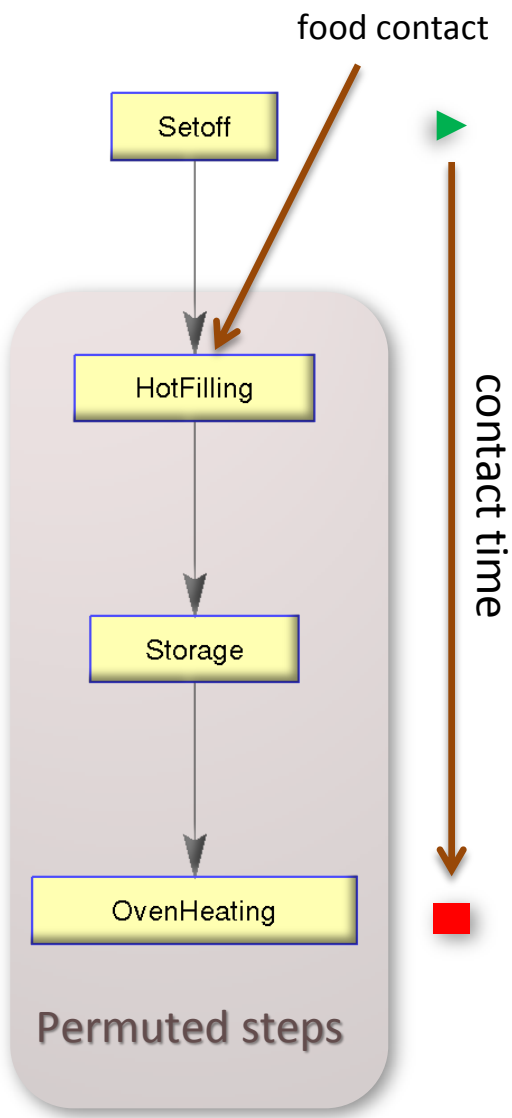
RESPONSABILITY ?

RULE 1: PERMUTING STEPS†
DOES NOT CHANGE THE FINAL MIGRATION



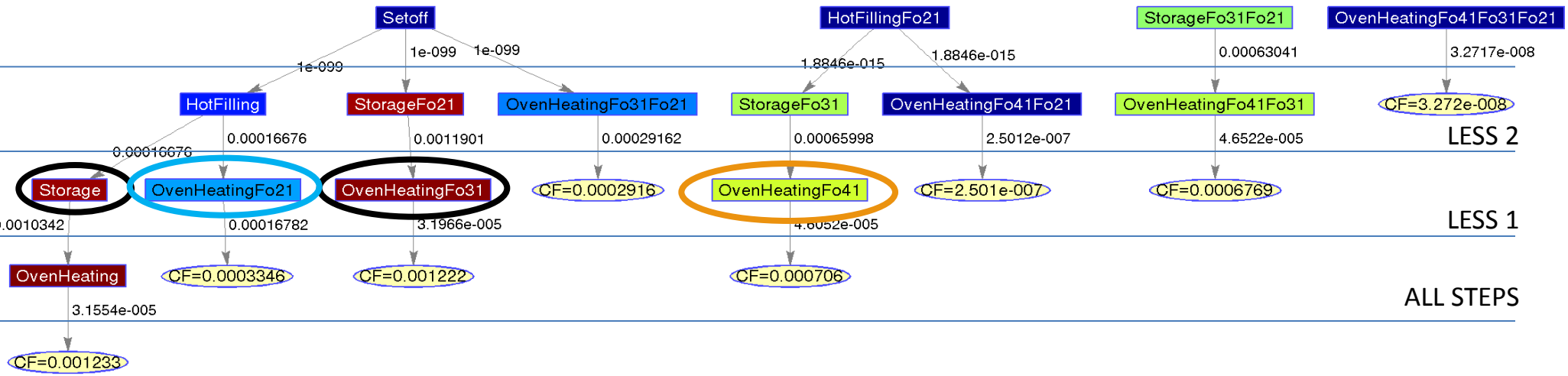
Name of last step

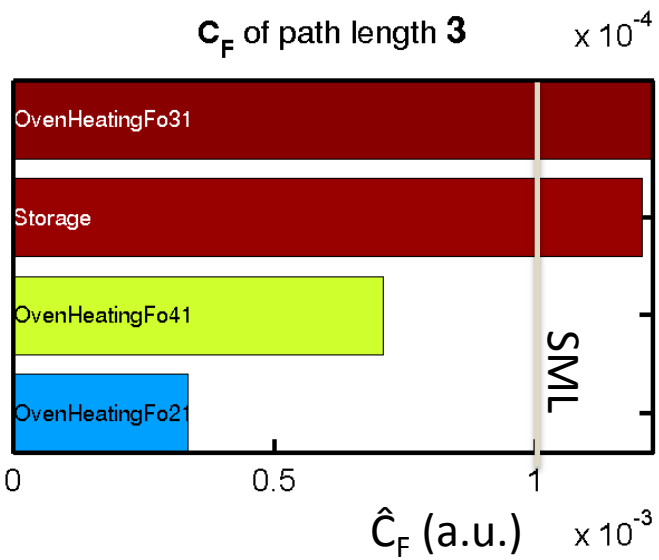
- OvenHeatingAS14
- StorageAS24
- OvenHeatingAS34
- HotFillingAS44
- StorageAS54
- HotFillingAS64



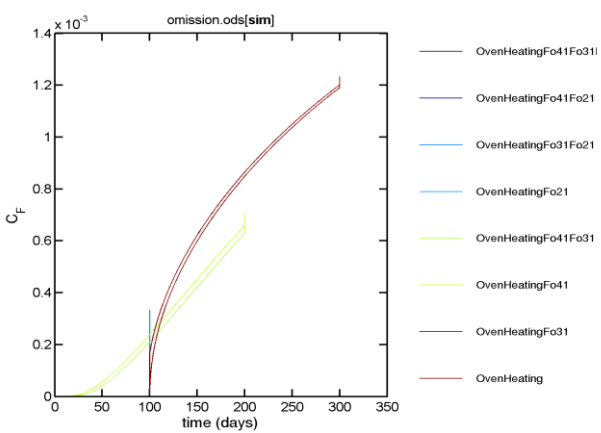
†For steps involving a contact with food

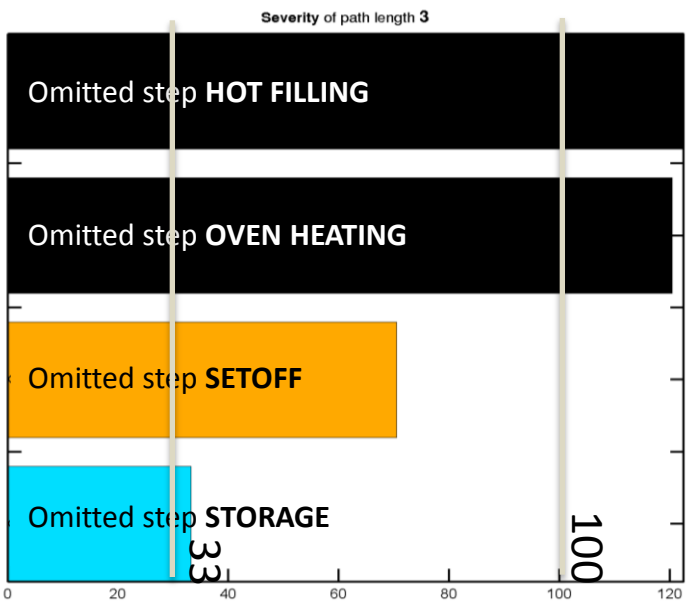
RULE 2: THE MODAL CRITICALITY ASSOCIATED TO ONE OR A COMBINED STEP(S) IS OBTAINED BY OMITTING THE STEP TO ASSESS



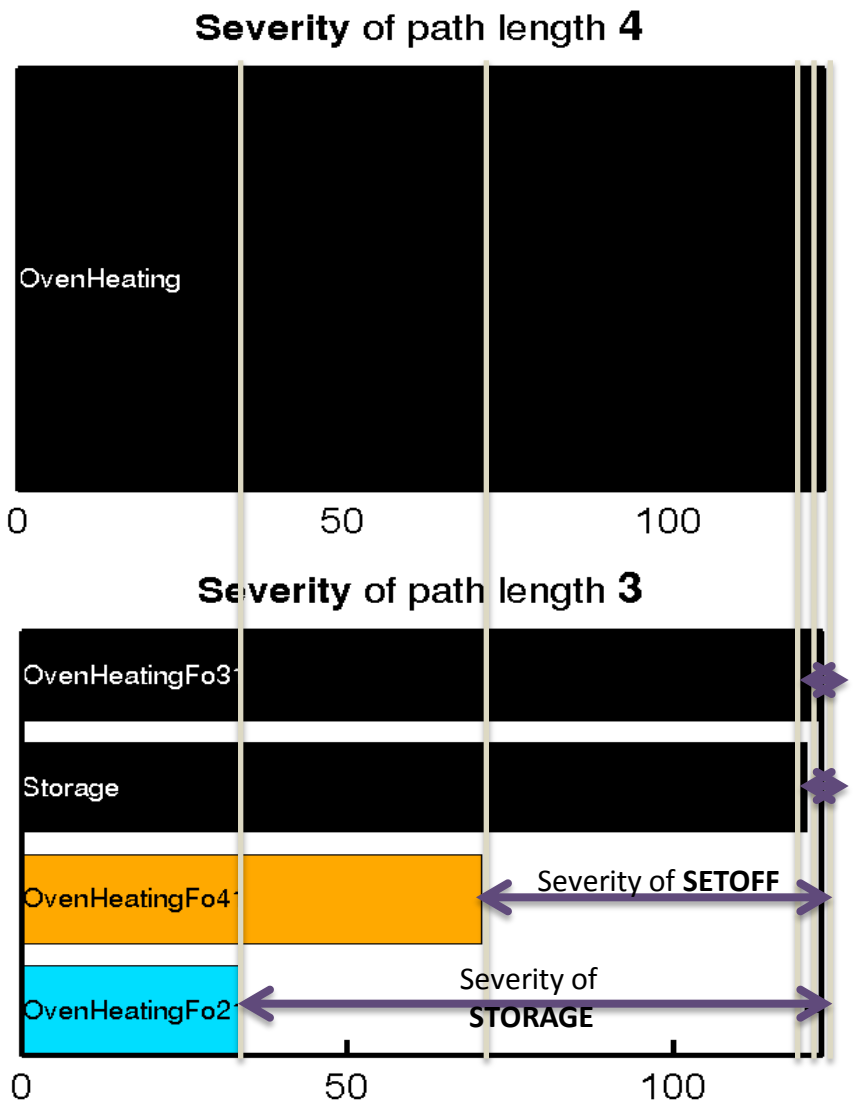


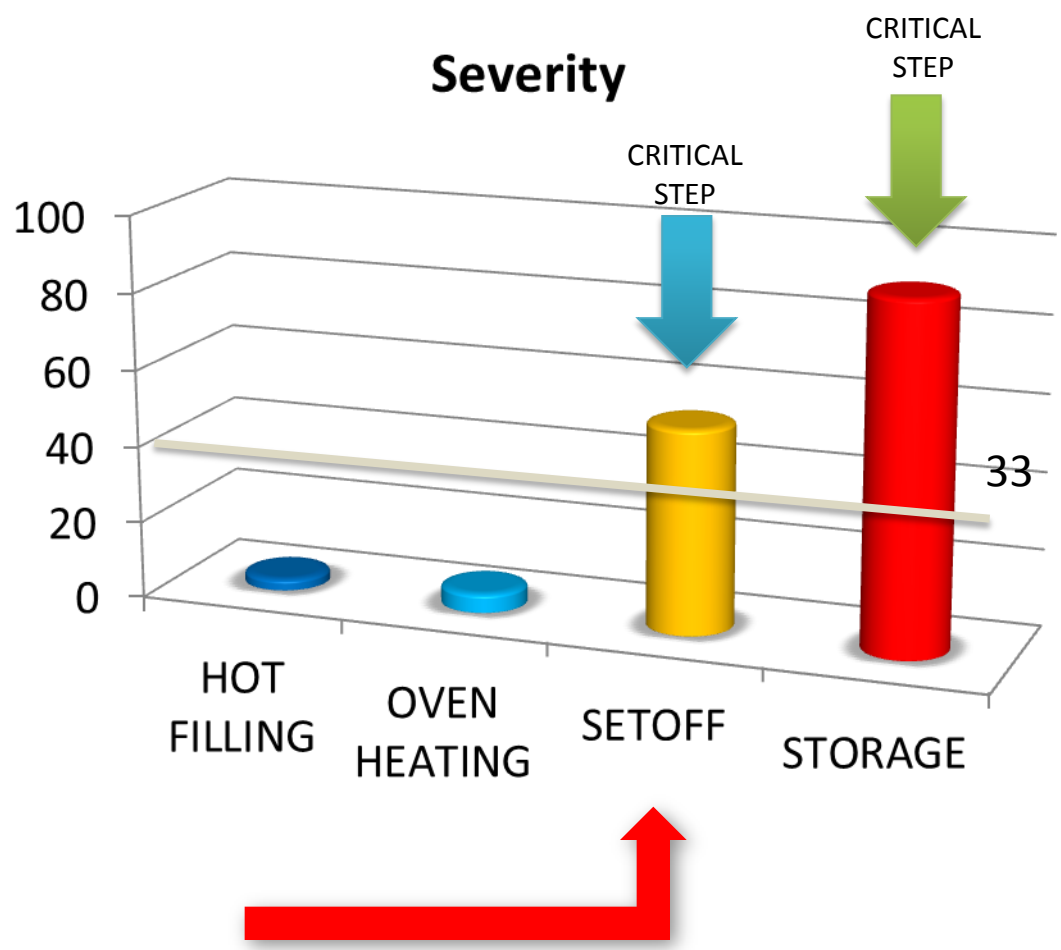
$\hat{C}_F$ → Severity





RULE 2: CALCULATION PROCEDURE TO EXTRACT THE SEVERITY OF A SINGLE STEP





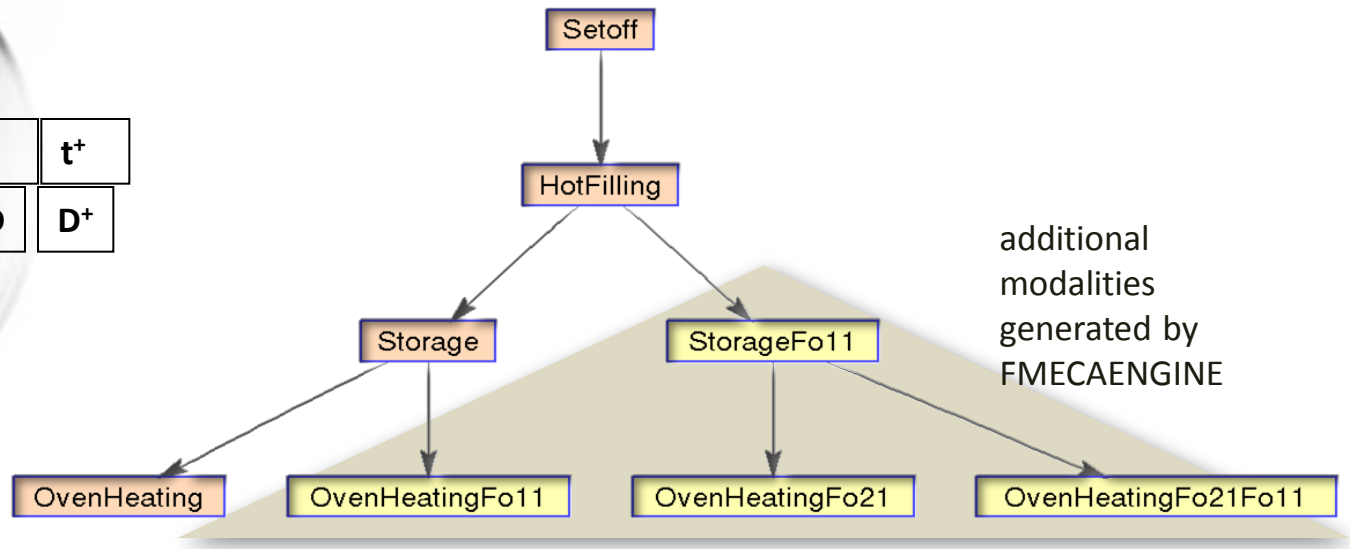
Severity(4 steps)-Severity(3 steps)

RULE 3: RATING COMBINED MODALITIES REQUIRES TO ASSESS THE CUMULATIVE EFFECT OF ALL COMBINATIONS (e.g. excessive storage and heating)

Storage : t and t^+

3	Storage	HotFilling	[1 10]	t	t^+
4	OvenHeating	Storage	[1 10]	D	D^+

Oven Heating : D and D^+



additional modalities generated by FMECAENGINE

JOURNEE_EMBALLAGE.ODS | 13-MAI-2011 14:46:03 | 15.2
KBYTES | C:\DATA\OLIVIER\AUDREY_GOUJON\MATLAB\TEST_ECHANGEABILITE\INPUTS

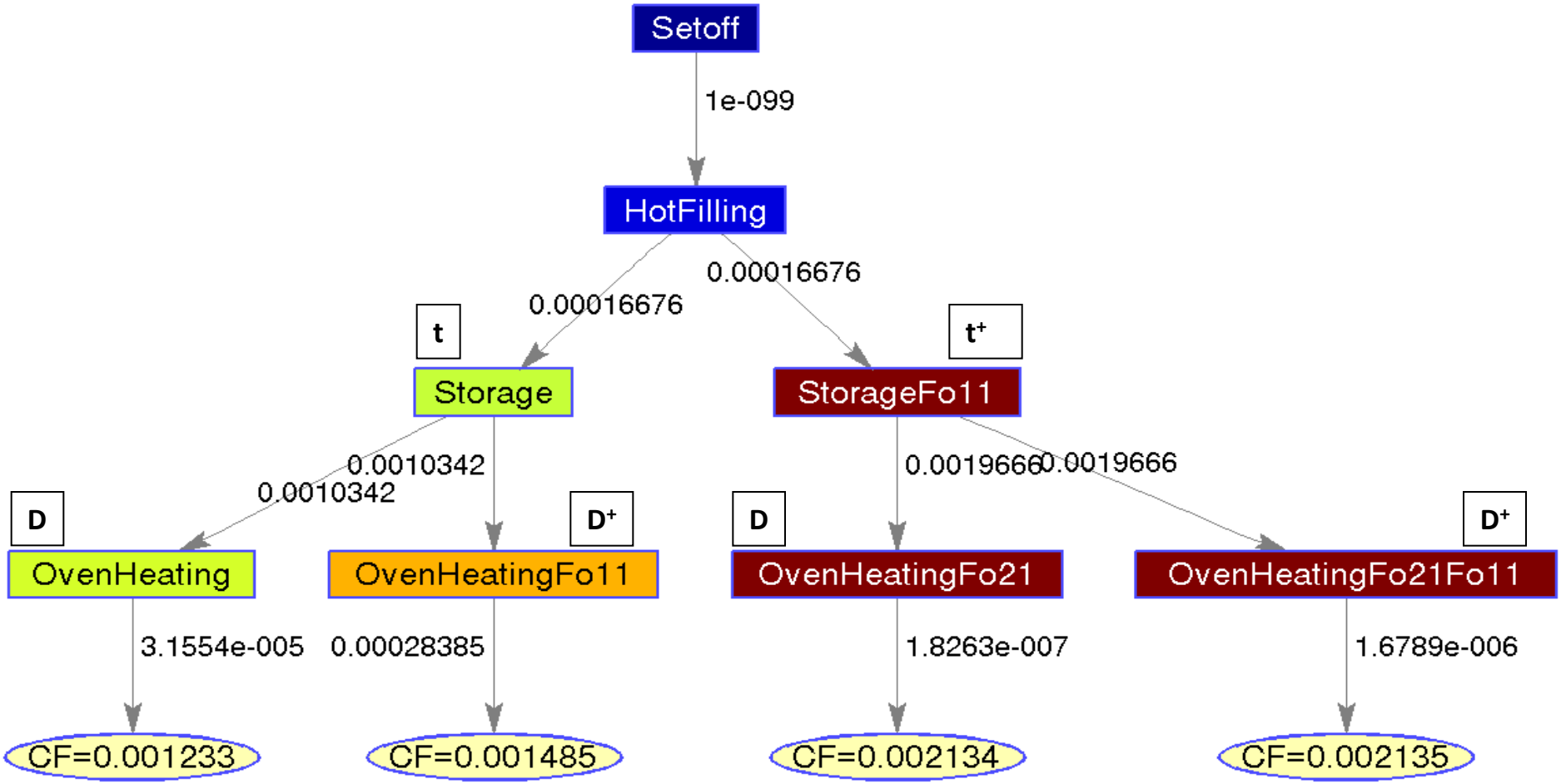
row	id	parent	Foscale	t	l_F	l_1	l_2	SML	CP_1^0	CP_2^0	Bi	D_1	D_2	KFP_1	KFP_2
row	*usercode*		*Foscale*	*s*	*m*	*m*	*m*	*kg/m³*	*kg/m³*	*kg/m³*	*no unit*	*m²/s*	*m²/s*	*(kg/m³)/(kg/m³)*	*(kg/m³)/(kg/m³)*
1	Setoff			8.64e+006	0.0115385	0.001	5e-005	0.001	0	0.5	-1000	3.3e-014	1.2e-016	10	1
2	HotFilling	Setoff		600							1000	1.77e-011	2e-013		
3	Storage	HotFilling	[1 10]	1.728e+007								3.3e-014	1.2e-016		
4	OvenHeating	Storage	[1 10]	300								1.1e-010	3e-012		

INPUT TABLE 4 simulation definitions date 13-May-2011 15:39:59

Missing values are inherited

RULE 3: RATING COMBINED EFFECTS

here: $tD < tD^{+} < t^{+}D < t^{+}D^{+}$

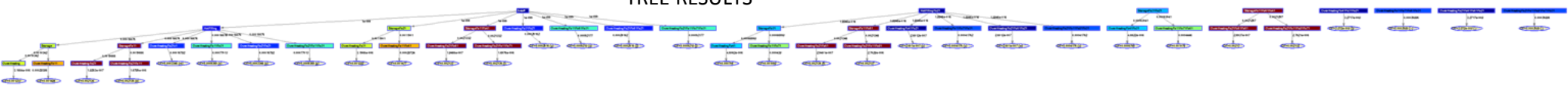


TO BE WEIGHTED BY EXPERTS

RULE 3: MODAL CRITICALITY ASSOCIATED TO [t,D] × [t⁺,D⁺]

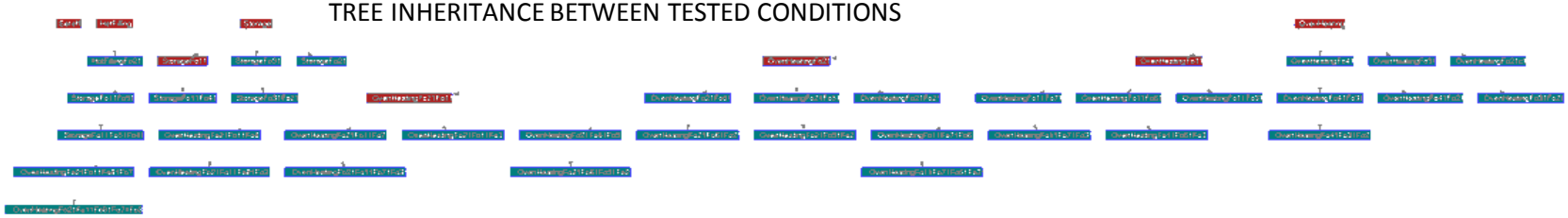
➔ all sequences with omitted steps (1..3) are tested (**43 simulations !**).

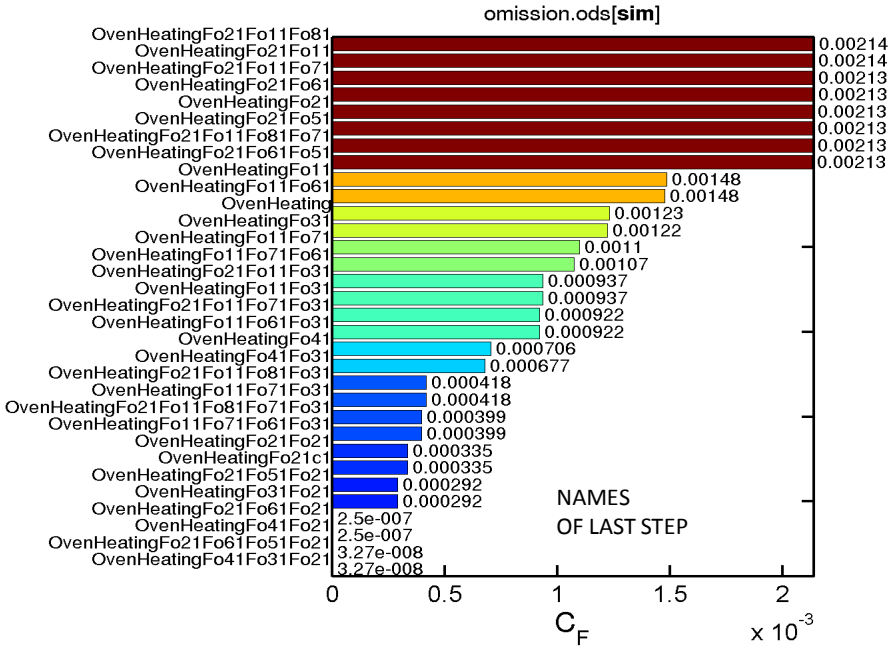
TREE RESULTS

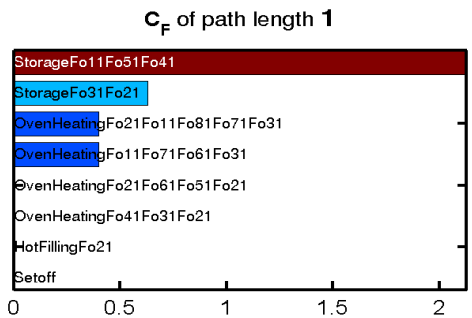


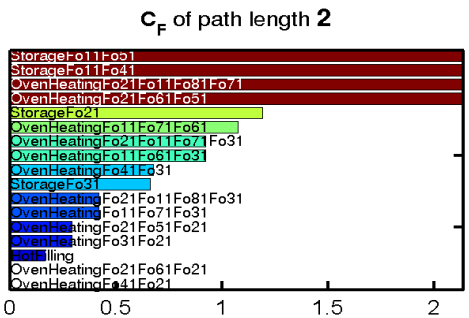
NAMES OF LAST STEP

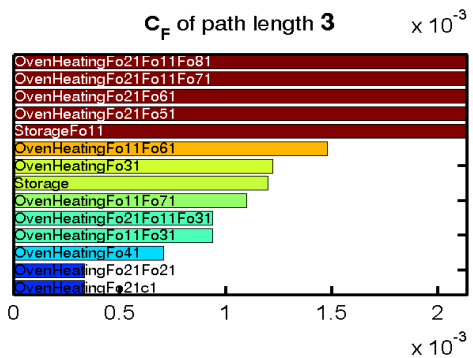
TREE INHERITANCE BETWEEN TESTED CONDITIONS

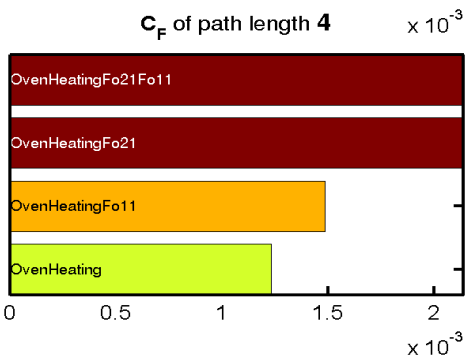






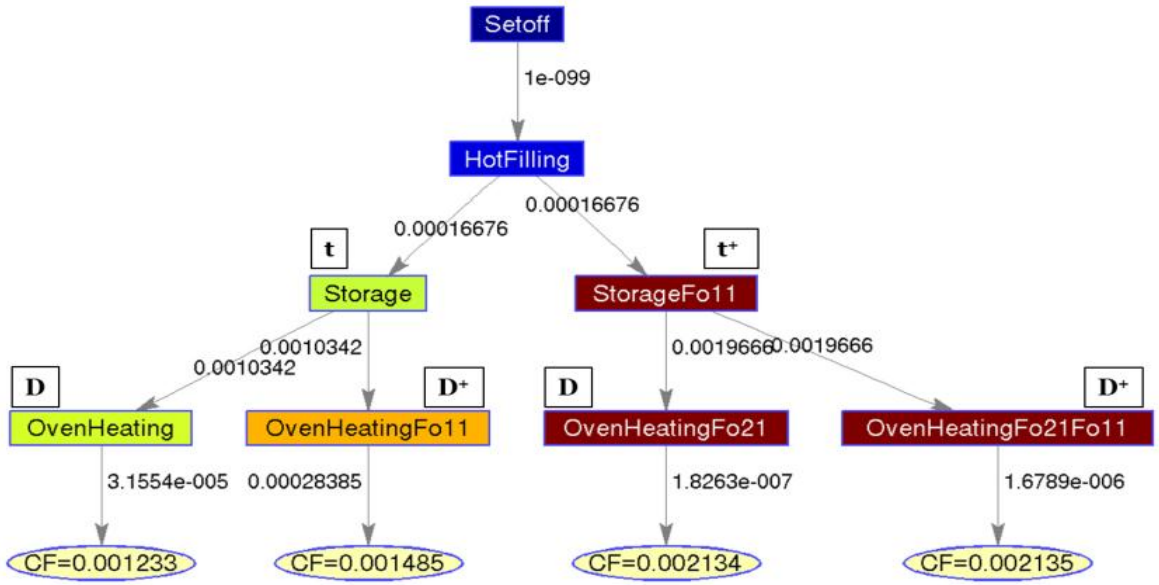


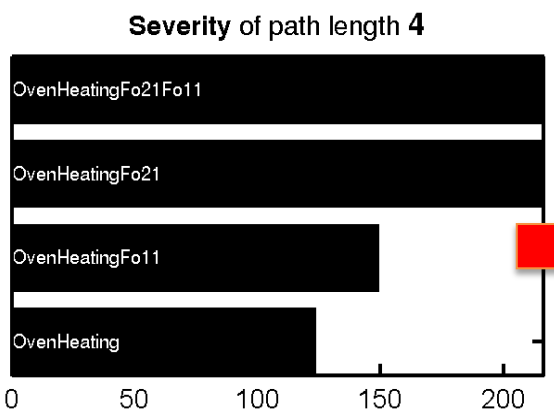


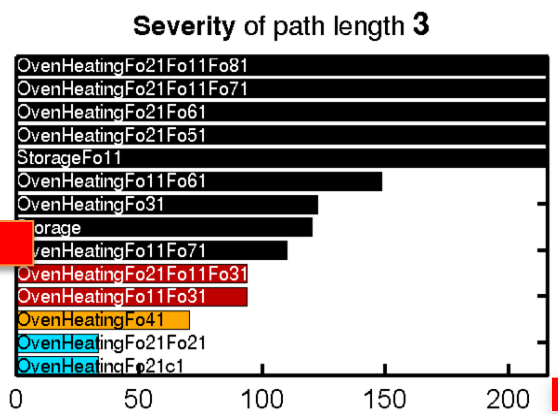


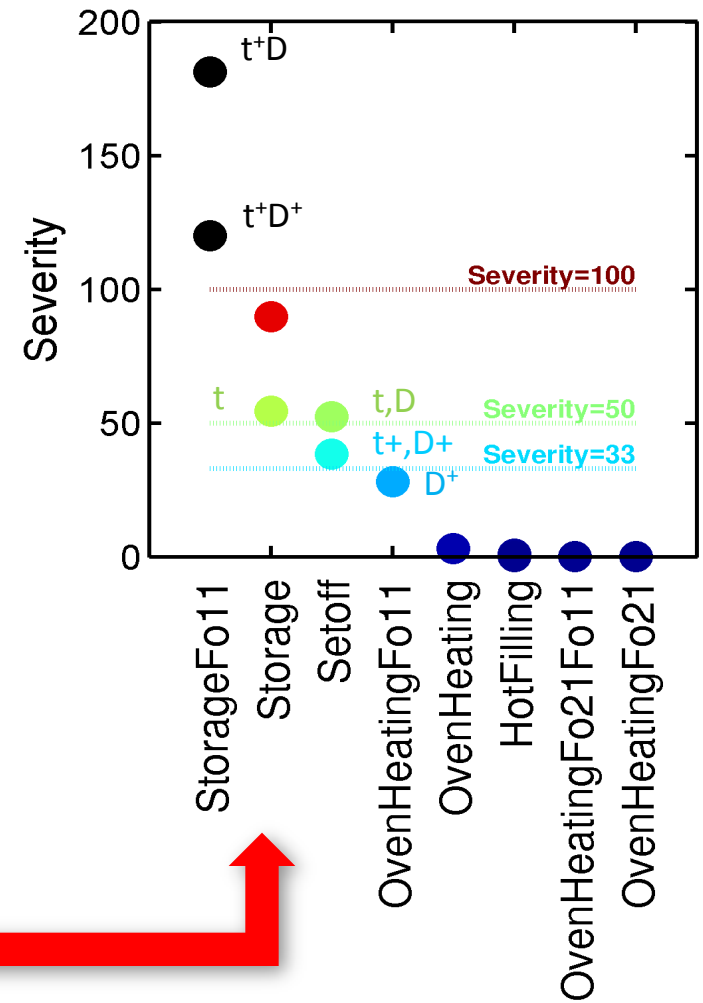
RULE 3: MODAL CRITICALITY ASSOCIATED TO [t,D] × [t⁺,D⁺]

➔ all sequences with omitted steps (1..3) are tested (43 simulations).





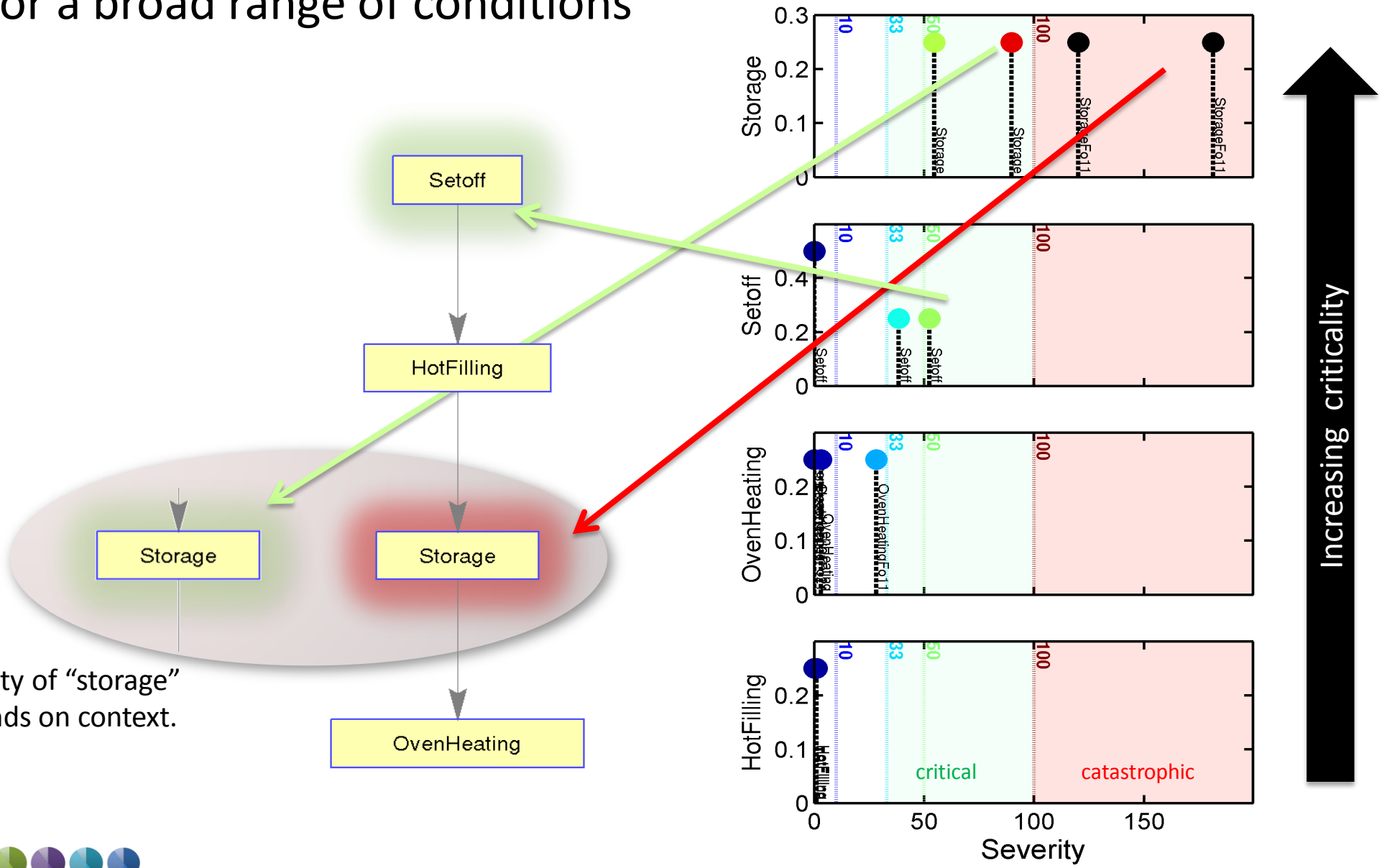




Severity(4 steps)-Severity(3 steps)

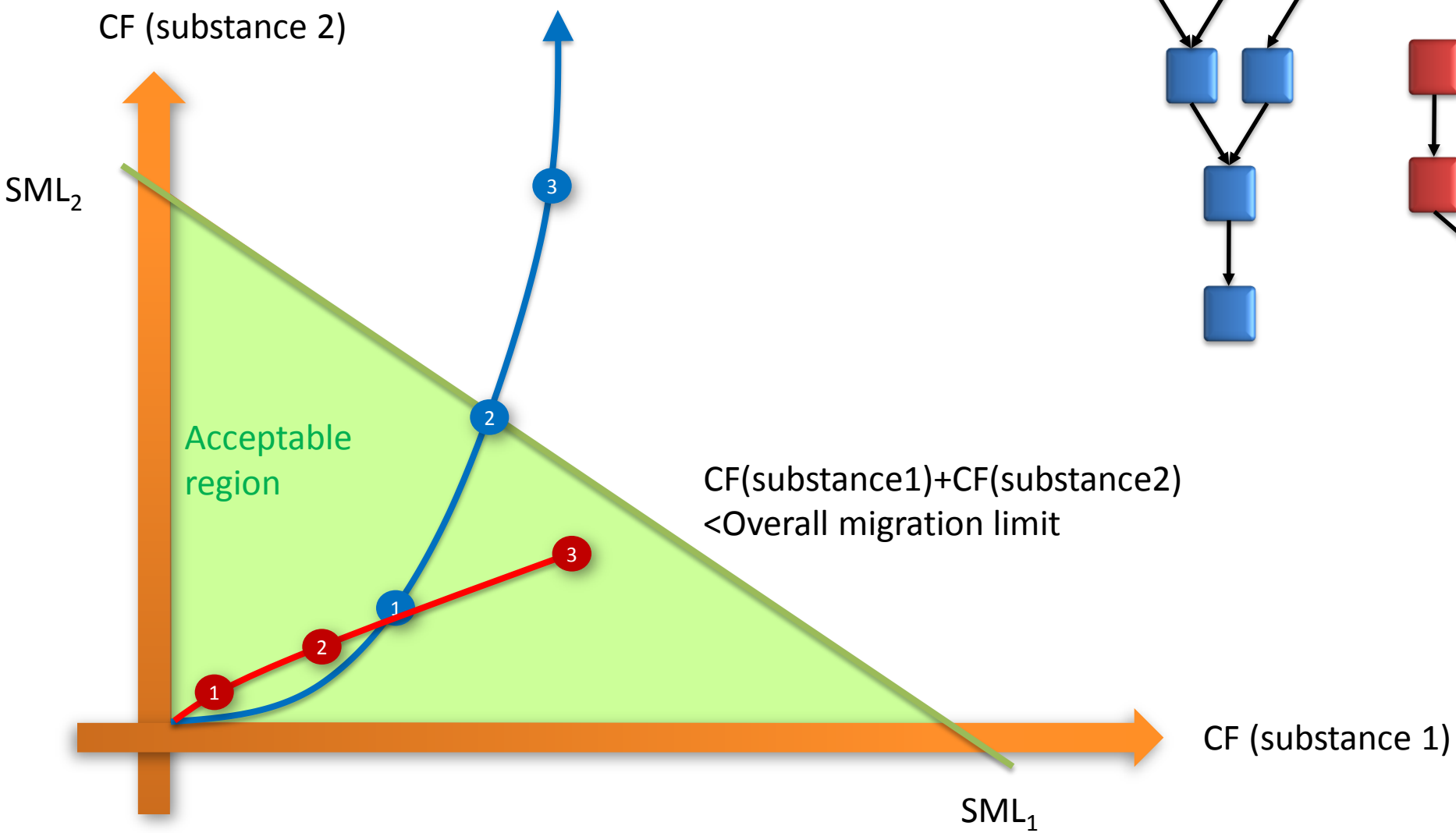
RATING SEVERITY

for a broad range of conditions



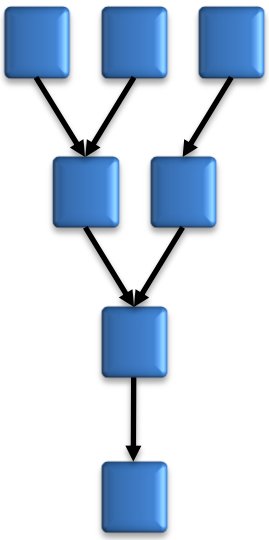
Severity of “storage” depends on context.

HOW DOES IT WORK?

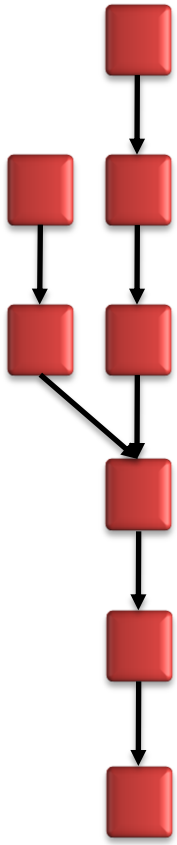


APPLICATION: CONCURRENT DESIGN/SCREENING

- DESIGN A



- DESIGN B

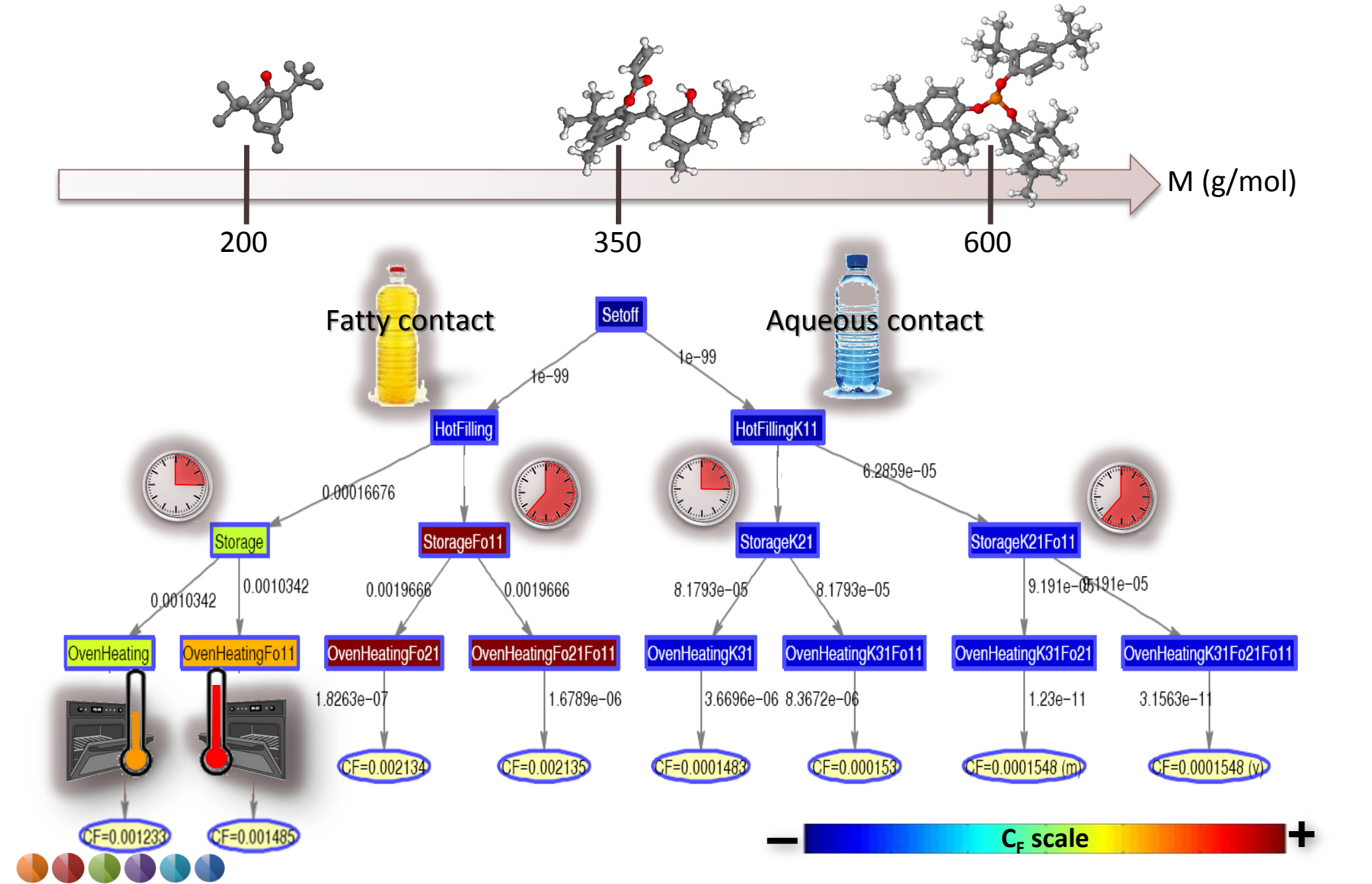


Identification of
- critical components
- critical steps
- uncorrectable design areas

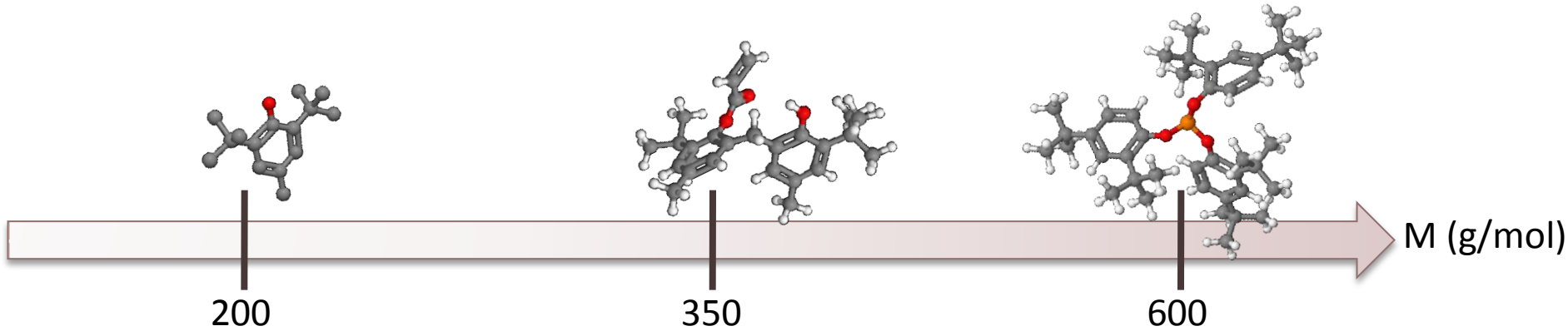
Feed results into
- Design
- Quality management procedures
- Suppliers audit

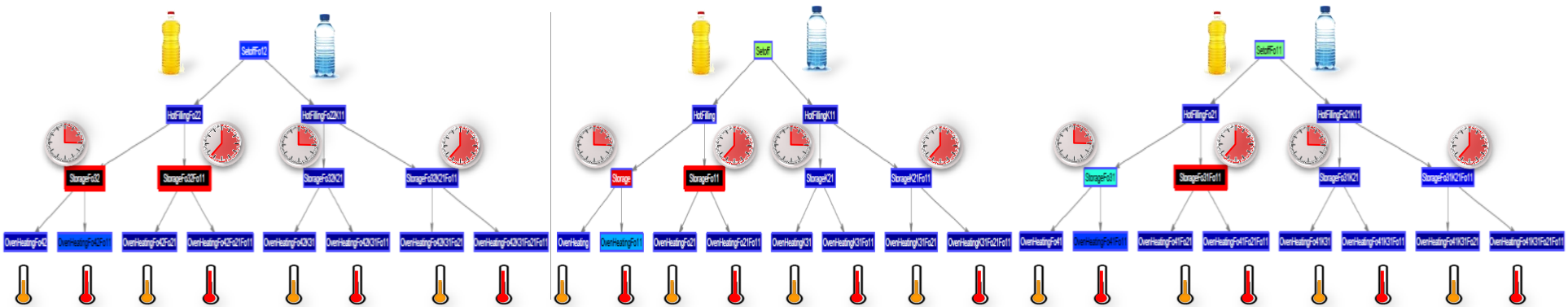
Considering related decisions

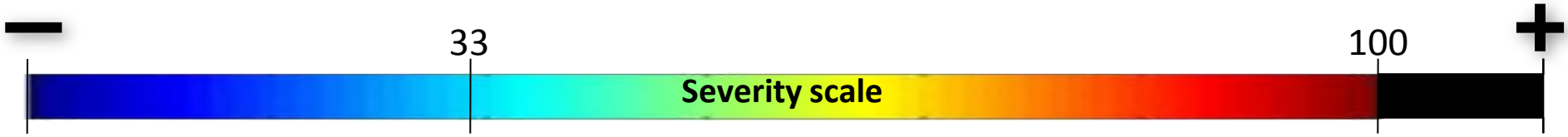
COMPLEX EXAMPLE OF COMBINED EFFECTS



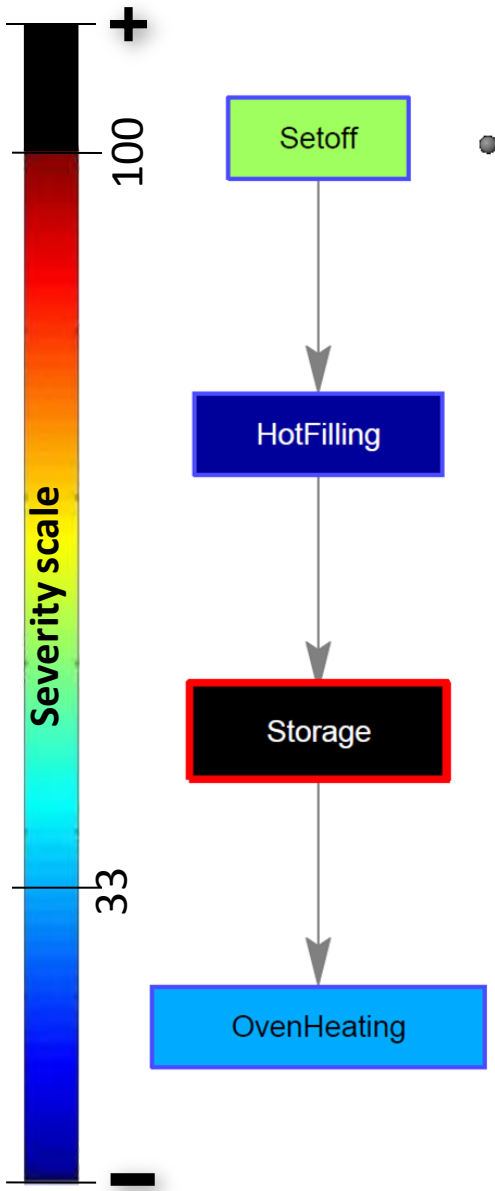
RATING SEVERITY for several migrants

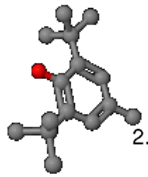


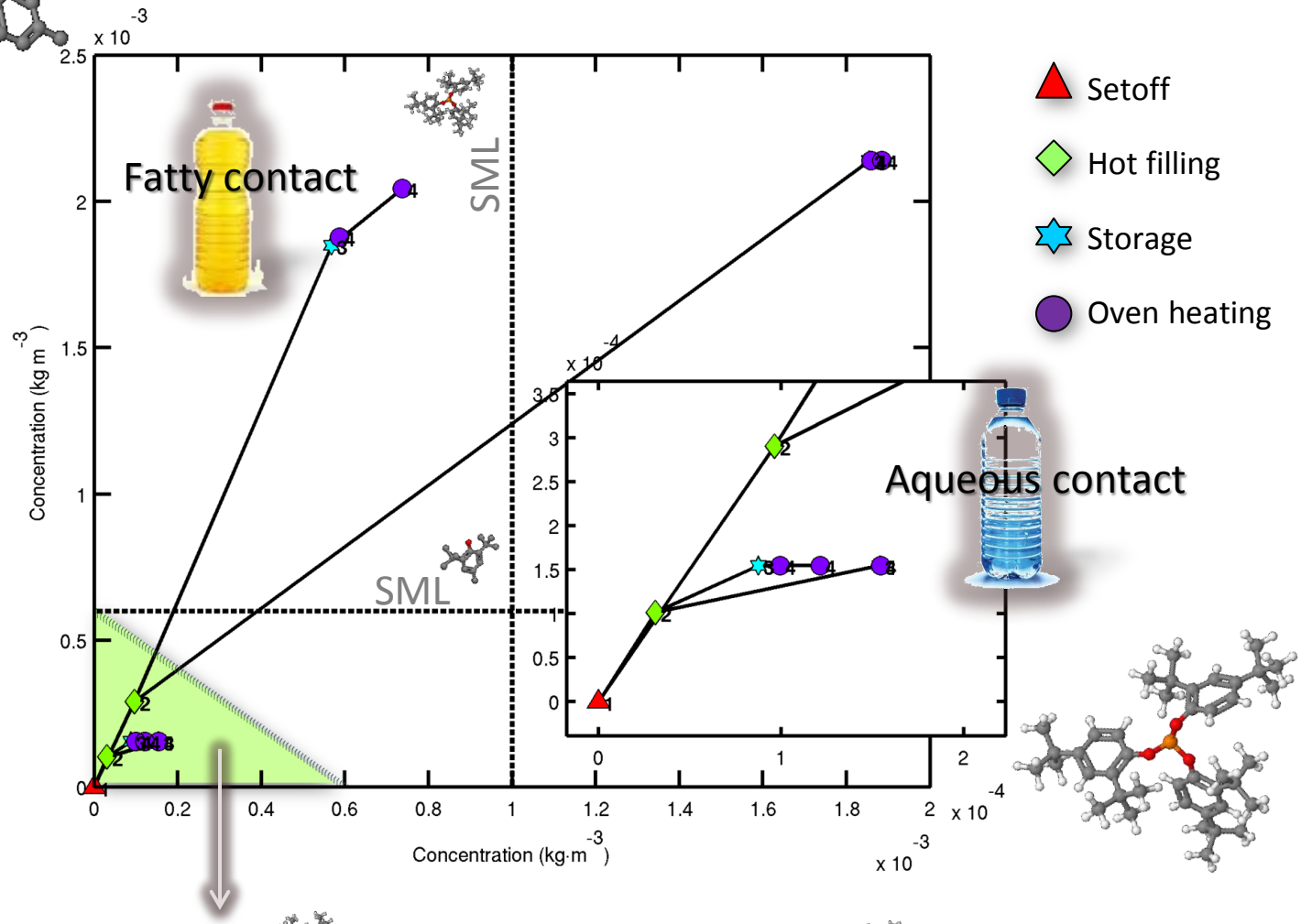




RISK BALANCING between migrants







$$C_F^{\bullet} + C_F^{\bullet} \leq \min\left(SML^{\bullet}, SML^{\bullet}\right)$$

CONNECTING WITH PHYSICO-CHEMICAL DATABASES

Relational databases

Key examples (coding with fmecaengine V 0.41 and later)

RELATIONAL DATABASES

Database = collection of tables including primary, super key and foreign keys

Examples

Monomer

Name
C_name
PMREF
CAS
M
SML
polymer
class

	A	B	C	D	E	F	G	H
1	name	C_name	PMREF	CAS	M	SML	polymer	class
2	4,4'-dihydroxy-2,2-diphenylpropar	bisphenol A	13480	80-05-7	228.29	0.6	PA	monomer1
3	Caprolactame		14200	105-60-2	113.16	15	PA	monomer1
4	Ethylene glycol		16990	107-21-1	62.07	30	PET/PEN	monomer2
5	1 butene		13870	106-98-9	56.11	60	LLDPE/HIF	monomer3
6	Ethylene		16950	74-85-1	28.05	60	LLDPE/LDI	monomer4
7	1-octene		22660	111-66-0	112.22	15	LLDPE	monomer5
8	Styrene		24610	100-42-5	104.15	60	HIPS/PS	monomer6
9	Terephtalic acide		24910	100-21-0	166.13	7.5	PET/PBT	monomer7
10	1-hexene		18820	592-41-6	84	3	HDPE/LLD	monomer8

monomer

Polymer

name
composition

	A	B
1	name	composition
2	HDPE	monomer4
3	HDPE	monomer8
4	HDPE	monomer10
5	HDPE	monomer11
6	HDPE	monomer12
7	HDPE	antioxidant
8	HDPE	UV_stabilizer
9	PP	monomer9
10	PP	antioxidant
11	PP	UV_stabilizer

polymer

Additive

name
PMREF
CAS
M
SML
Class

	A	B	C	D	E	F
1	name	PMREF	CAS	M	SML	class
2	-tert-butyl-4-	46880	65140-91-2	694.84	6	antioxidant
3	s(6-tert-butyl	66480	119-47-1	340.5	1.5	antioxidant
4	is(4-ethyl-6-t	66400	88-24-4	368.55	1.5	antioxidant
5	is(6-tert-buty	92800	96-69-5	358.54	0.48	antioxidant
6	i-tert-butyl-4	59200	35074-77-2	638.93	6	antioxidant
7	bis(3-(3,5-di-	70000	70331-94-1	696.91	60	antioxidant
8	peridine-succ	60800	65447-77-0	1500	30	UV_stabilizer
9	methylpheny	60400	3896-11-5	315.8	30	UV_stabilizer
10	-n-octyloxybe	61600	1843-05-6	326.5	6	UV_stabilizer
11	4,6-bis(1-met	60320	70321-86-7	447.58	1.5	UV_stabilizer

additive

Affinity

food
K

	A	B
1	food	K
2	aqueous	0.001
3	fat	1
4	dairy	1
5	dairy	0.001

affinit

IMPLEMENTED RELATIONSHIPS

Implemented relationships include:

- one-to-one relationships
- one-to-many relationships
- many-to-many relationships
- cascading between keys

Operations above are coded using a special syntax (more flexible and concise than SQL) that mimics UML (http://en.wikipedia.org/wiki/Unified_Modeling_Language) :

PP:polymer::name->classadditives
PP:polymer::name->classadditives:substance::class->name
PP:polymer::name->classadditives:substance::class->M

By default, a UNIQUE operator operator (data reduction) is apply to all relationships involving strings or cell array of strings. The request order is respected only for single requests.

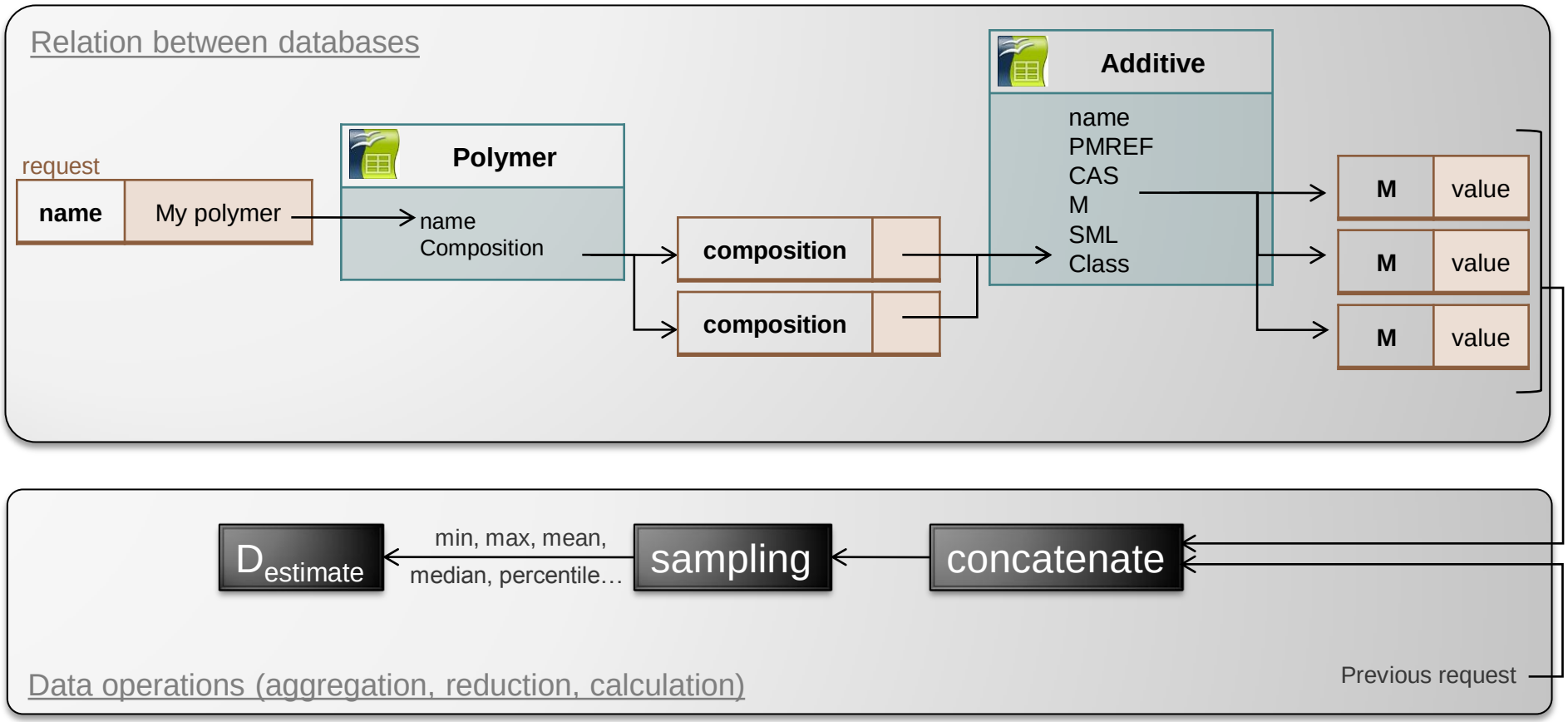
It is worth to notice that final results are also included within a large database that can be resused in future simulations or in subsequent analysis (e.g. for calculating severity).

Background:

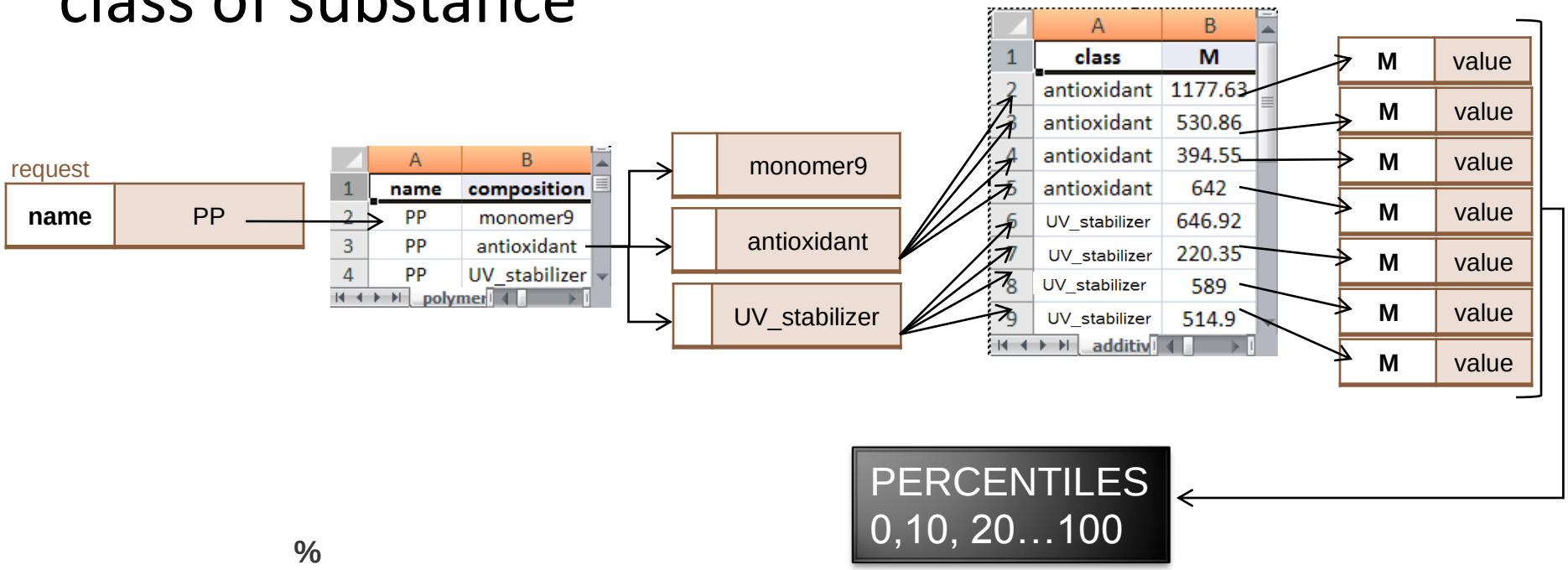
http://en.wikipedia.org/wiki/Many-to-many_(data_model)
http://en.wikipedia.org/wiki/Junction_table
http://en.wikipedia.org/wiki/Foreign_key
http://en.wikipedia.org/wiki/Superkey
http://en.wikipedia.org/wiki/Associative_Entities

EXAMPLE OF **ONE TO MANY** RELATIONSHIPS

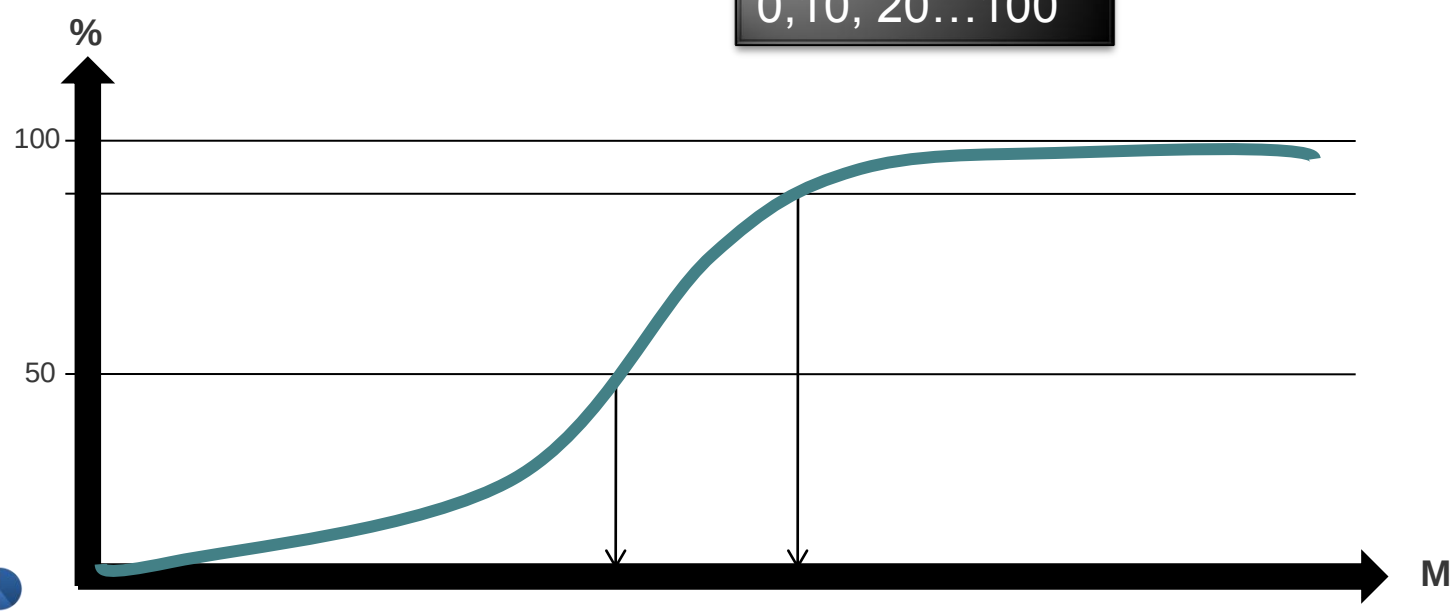
The example depicts how databases could be used to derive the formulation (substance content) of a common polymer and finally to sample the distribution of molecular mass (M) of possible migrants. These values are finally used for the calculation of some estimates of diffusion coefficients (D).



TIP: the name of a substance can be replaced by a class of substance



PERCENTILES
0,10, 20…100



RELATIONSHIPS are called KEY or KEY-to-KEY

KEY2KEY syntax

Basic coding

- keyA:tableA::columnA1->columnA2
- keyA:tableA::columnA1->columnA2:tableB::columnB1->columnB2
- keyA:tableA::columnA1->columnA2:tableB::columnB1->columnB2:tableC::columnC1->columnC2

Extended coding with mathematical operators

- max(Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M,40))
- Dpiringer(PP,min(PP:polymer::name->classadditives:substance::class->M),40)

Extended coding with regular expressions

- \antiUV{3|2}\ :substance::name->M
- \.#PE.#\:polymer::name->classadditives:substance::class->name:substance::name->M

Extended coding with lists

- LDPE|undefined|PP:polymer::name->classadditives:substance::class->name:substance::name->M

EXAMPLES

Collection of D

Dpiringer(PP,PP:polymer::name→composition:additive::class→M,25) ➔ D_{min}, D_{med}, D_{max}

Dpiringer(PP,min(PP:polymer::name→composition:additive::class→M,25))
ou
max(Dpiringer(PP,PP:polymer::name→composition:additive::class→M,25))

} D_{max}

Collection of K

dairy:affinity::food→K ➔ K_{min}, K_{med}, K_{max}

Collection of SML

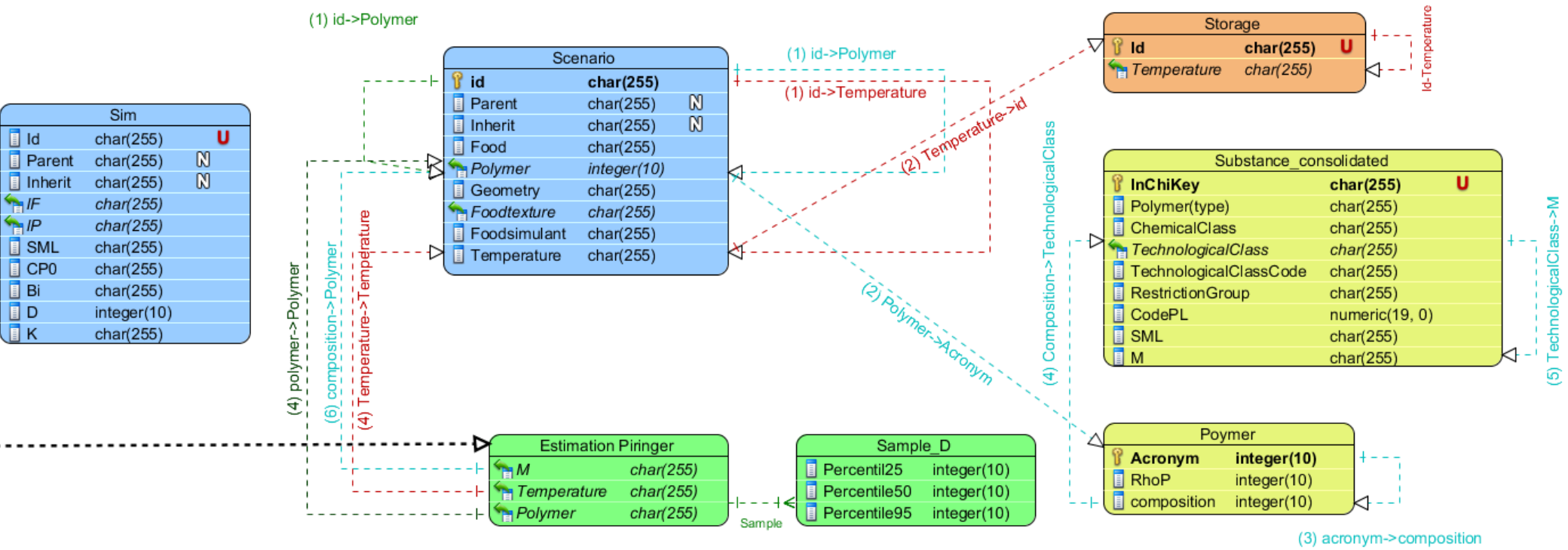
mean(PP:polymer::name→composition:additive::class→SML) ➔ SML_{mean}

➔Any valid Matlab expressions can be accepted

EXAMPLE with multiple keys

note that all keys must be enclosed within ()

Dpiringer((LDPEYogurtBottle:scenario::id->polymer),
(LDPEYogurtBottle:scenario::id->polymer:polymer::acronym->composition:substance::technologicalclass->M),
(LDPEYogurtBottle:scenario::id->temperature:storage::id->temperature))



HOW TO BUILD USER DATABASES, RULEBASES, KNOWLEDGEBASES

Database, rulebase, knowledgebase = collection of tables including primary, super key and foreign keys

Examples: Tables of physico-chemical properties

Additive	
InChIKey:*string (U)*	NLZUEZXRPGMBCV-UHFFFAOYSA-N
Name:*string*	2,6-Di-t-butyl-4-hydroxytoluene;2,6-di-tert-butyl-4-methyl phenol;4-Methyl-2,6-bis(2-methyl-2-propanyl)phenol;4-Methyl-2,6-di-t-butyl-phenol ;4-Methyl-2,6-ditertbutylphenol;BHT;Butylated hydroxytoluene;phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl;2,6-Di-t-butyl-p-cresol
CAS:*list of strings*	128-37-0;1948-33-0;25377-21-3;50-78-2;62698-56-0;720-39-8;950-56-1;97123-41-6
PMREF:*integer*	46640
M:*real*	220.35
SML:*real*	3
TDI:*real*	**0.05**
logP: *real*	5.2
logPmin: *real*	5.32
logPmax: *real*	5.03
Class:*string*	Antioxidant

Monomer	
InChIKey:*string (U)*	QQONPFPTGQHPMA-UHFFFAOYSA-N
Name:*string*	name: propene;1-propene;propylene;methylethene;1-propylene;prop-1-ene
CAS:*list of strings*	115-07-1;33004-01-2;676-63-1
PMREF:*integer*	23980
M:*real*	42.08
SML:*real*	60
TDI:*real*	NaN
logP:*list of reals*	1.7
Class:*string*	propylene
Polymer:*string*	PP

Polymer	
Acronym:*string*	PP
Name:*string*	polypropylene
Class:*string*	PO
Density:*real*	0.95;0.92
Composition: *list of strings*	antioxidant, UV_stablilizer, monomer

ALL DATA TYPES ARE RECOGNIZED IMPLICITELY ACCORDING TO THE FOLLOWING RULES	
Empty cell	= Not A Number
Scalar	Any numeric value
List	String containing “;” or “|”
Unique (U)	is enforced for all keys returning an array of strings
Primary/Foreign key	Any key with string/char content (possibly including some lists)

EXAMPLES: RULE BASES AND KNOWLEDGE BASES

scenario	
Primary key	**Id:** gobeletPP
Foreign key	**Food :** hotdrink
List/Foreign key	**Foodsimulant:** fatty, ethanol50
Foreign key	**Material :** PP
Foreign key	**Geometry :** gobelet
Foreign key	**Step** : consumption
Foreign key	**Temperature :** hot

Food	
Primary key	**Id:** hotdrink
List/ Foreign key	**Shelflife**: 2
List/ Foreign key	**Shelflifeunit :** h
List/ Foreign key	**rhoF**: 1000

Consumption	
Primary key	**Id :** hot
List/ Foreign key	**Temperature:** 70
List/ Foreign key	**Time:** 2
List/ Foreign key	**Unit:** h

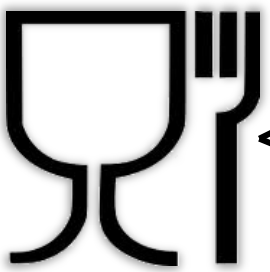
Geometry	
Primary key	**Id:** gobelet
List/ Foreign key	**A:** 170
List/ Foreign key	**Aunit:** cm2
List/ Foreign key	**mF:** 200
List/ Foreign key	**mFunit:** g
List/ Foreign key	**lP :** 150
List/ Foreign key	**lPunit** : µm

Foodsimulant	
Primary key	**Id:** ethanol50
List	**K:** 0.1

Diffusion	
Primary key	**InChIKey**: NLZUEZXRPGMBCV-UHFFFAOYSA-N
	M: 220.35
	polymer: PP
	rhoP: 0.95
List	**temperature**: 40
	D: 4.6E-15;2.7E-16;5E-15

POSSIBLE EXTENSIONS

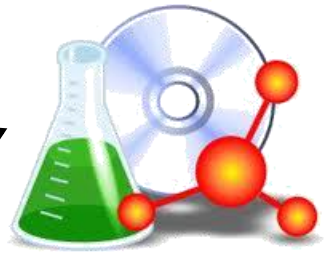
Positive lists



AUTOMATIC TOOL TO IMPORT

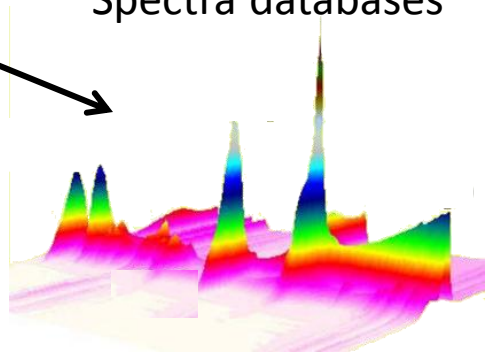
AUTOMATIC TOOL TO IMPORT

Physicochemical properties



NIST
Ncbi
ChemSpider
PubChem
EPA…

Spectra databases



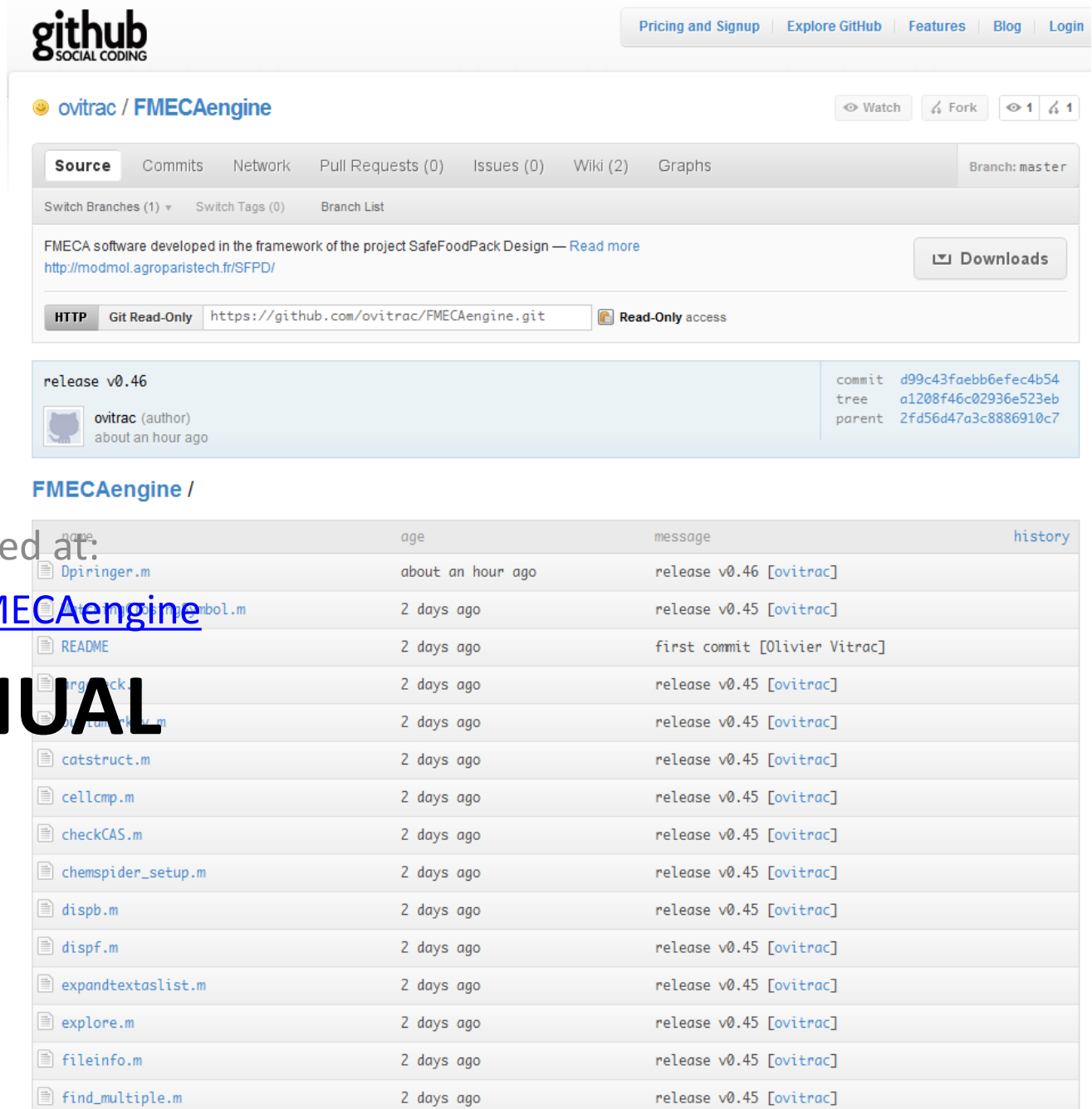
Building of the first substances database

- M
- SML
- TDI
- logP
- $T_{boiling}$
- $T_{melting}$
- Spectra :
  - -UV-V
  - -IR
  - -RMN
  - -Mass
- Chromatogram
- etc…

All functions can be downloaded at:

https://github.com/ovitrac/FMECAengine

DETAILED MANUAL



fmecaengine

```
fmecaengine: advanced script/function (object-oriented) to launch complex FMECA calculations from an OpenOffice Spreadsheet

   USAGE AS A SCRIPT (depreciated)
   Once the section "path and file definitions" properly defined, you need only to press F5 (i.e. run)
   To override default values, define user variables in the workspace

   USAGE AS A FUNCTION (recommended)
     Syntax: fmecaenfine('variable1','value1','variable2','value2','variable3','value3',...)
             fmecaenfine(definition,...) whith definition a structure with fields definition.variable1 = 'value1'

   LIST OF USER VARIABLES
               local  root directory of all files and folders (default = pwd)
           inputpath  folder that contains all inputs (relative to local, default = 'inputs')
          outputpath  folder that contains all outputs (relative to local, default = 'outputs')
       fmecamainfile  filename of ODSfile (located in inputpath, default = 'fmeca_demo.ods')
                      a structure (matching the output data0) can be used instead to link several calls of fmecaengine (use inputpat
                      setup the pattern for output filenames, it must include an )
          fmecadbfile  fmecadbfile of the meta database (default = 'fmecabaseofconditions.mat')
       fmecasheetname  name of spreadheet that (default = 'sim')
                      If you use several sheets, do not use same id between sheets as it will be break the consistency of simulation
             database  a database to feed all numeric input values (with statistics if needed) including Foscale, Kscale
                      a structure such database.table.column than can be indexed as valueA:table::columnA->columnB
                      a valid ODS file that code for a similar structure (table=sheetname, column names=first row)
                      By default, fmecaengine assumes that fmecamainfile is a such database
             severity vectorized anonymous function to define severity (default = @(CF,SML) 100*99./max(100*SML./CF-1,0))
                     Alternative, define first NOELfact = 100;
                     @(CF,SML) NOELfact*(NOELfact-1)./max(NOELfact*SML./CF-1,0)
               sample anonymous function to setup how a one->many or a many->many relationship is sampled
                      default = @(x) prctile(x,[5 50 95]) (only 5th, 50th and 95th percentiles are consideredà
                      versions older than 0.43 used @(x) [min(x) median(x) max(x)]
                      Note that Foscale and Kscale derived from one->many or a many->many relationships are normalized from the medi
                      the sample: setdiff(sample,median(sample))/median(sample)
   ADDITIONAL PROPERTIES FOR ADVANCED USERS (change solver performances used in senspatankar and variants, enable linked instances o
             nograph flag value (default=true) to prevent graphs from being plotted
             options ODESET structure
                     default value = odeset('RelTol',1e-4,'AbsTol',1e-4,'Initialstep',1e-8,'Maxstep',1e3,'Maxorder',2); % note based
               nmesh number of finite volumes for a layer with a dimensionless thickness of 1 (accurate for most of purposes)
                     default value = 200
       fmecamainfile  matching the output structure data0 can be used instead of a filename to link several calls of fmecaengine
           inputpath (when fmecamainfile is a structure) setups the pattern for output filenames (it must include the extension .ods

   OTHER PROPERTIES (to change the behavior of fmecaengine, mainly for developers, see code for additional details)
             headers number of header lines (default=2) in fmecamainfile:fmecasheetname
     databaseheaders number of header lines (default=1) in database file
           regular_l, regular_D, regular_K, regular_C:
                 regular expressions to identify column titles matching l,D,K,C
           print_id, print_parent, print_inherit, print_l, print_D, print_K, print_C, print_t, print_L, print_Bi:
                 expressions (matching fprintf syntax) to name layers id,parent,inherit,l,D,K,C,t,L,Bi

   OUTPUTS
   fmecadb = fmecaenfine(...) returns the global database listing all conditions
   [fmecadb,data0,data,options] = fmecaenfine(...) returns the input parameters as a structure
       data0: initial content of fmecamainfile as a structure
        data: state of data0 after execution of fmecaengine
     options: options used in the current instance of fmecaengine

   OUTPUT FILES (located in outputpath)
       raw MAT files for post-processing
       HTML report with linked PNG and PDF files (individual simulations, dependence/inheritance/result graphs, Pareto charts)

 DETAILED DESCRIPTION
 > The current script reads the spreadsheet 'sim' from an ODS file (OpenOffice Spreadsheet) to setup complex migration simulations.
 > Possible simulations (possibly combined) include: multilayer, chained scenarios, setoff effect, hot-filling, sterilization...
 > Titles in the spreadsheet are used to recognize variables/inputs.
 > Please, check closely the structure of the demonstration ODS file (fmeca_demo.ods) before using this script.
 > Each row in the spreadsheet codes for a single simulation. The spreadsheet can contains an arbitrary number of rows.

 > A column "id" is used to identify each simulation inputs and outputs.
 > Complex chaining of simulations is enabled by using the column "parent" that gives the id of the previous result
   to be used as input for the next simulation.
   The script does not post-process the simulations. It stores all intermediate simulations results as a MAT file (id.mat).
   For routine control, a corresponding id.png and id.pdf, including the concentration profile and concentration cinetic
   with twice the requested time, are also saved together.
   A metadatabase 'fmecadb' (data about simulations), whose filename is defined by the variable fmecadbfile, stores all
   simulation conditions including solver parameters.

 > The script manages the prioritization and history of all simulations regardless their order in the spreadsheet and
   their chaining complexity (only limitation: a single parent).

 > For dependent simulations, default input inheritence is also accepted so that only modified parameters need to be specified
   and all other variables/inputs can be left empty.
 > The script detects any change in unputs and restart all dependent simulations in cascade.
 > Removing any id.MAT file or the entire output directory forces corresponding simulations to be restarted.
 > Removing an entry id in 'fmecadb' (with the command rmfield) is the same as removing the corresponding id.MAT
   (the corresponding MAT file will be rewritten).

 > Inheritance of the sole inputs (while discarding simulations results) is possible via an optional column 'inherit'.
   All empty or NaN cells are replaced by their equivalent contents from the row with id corresponding to 'inherit'.
   Complex propagation are allowed for inheritance (e.g. cascading, tree) whatever the dependence enforced by parent.
   In case of conflicts between inputs inheritance between 'parent' and 'inherit', the later have a higher precedence.
   As a rule of thumb, use 'parent' to chain simulations and prefer 'inherit' for sensitivity analysis
   (e.g. to calculate Jacobians).
```

```
> Combinatory simulations (Full or pseudo Monte-Carlo [preferred]) are setup via special columns that contain vectors of scaling va
  A valid Matlab syntax embedded with a string can be used to define vectors (1:3, [.1 10], logspace(-3,3,10) ...)
  Note that the scaling value 1 is removed from the list as the original row with defined values is considered to be
  the reference simulation with a unitary scaling (i.e. no scaling).
  Tree bifurcations/ramifications induced by multiple values are automatically generated. New id are based on original
  id by combining the name of scaling variable (e.g. Fo or K) the following tree level (1..m) and the scaling value (1..n).
  Row vectors (e.g. 1:3) do not propagate scaling values to children (to simulate different contact times at a step).
  Column vectors (e.g. (1:3)') propagate scaling values to children (to simulate different classes of molecules).
  Currently, the following scaling parameters are recognized:
      Foscale scale to simulate indifferently variable diffusion time and diffusion coefficients
      Kscale to simulate different chemical affinity.

> To assess the effect of a single setup, use 0 as scaling parameter (non-propagable value). The corresponding step
  will be removed. When required, new roots are added to the simulation tree.

  fmecaengine can be linked with internal and external databases with keyword 'database' and relational syntaxes (see KEY2KEY).
  EXAMPLES for fmeca_demo3.ods:
   100*(test_key:sim::id->CP20) to reuse the concentration value of the simulation with the id test_key
   1000*min(PP:polymer::name->classadditives:substance::class->SML) replacing a numerical SML value
   min(Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M,40)) replacing a numerical D value
   Dpiringer(PP,max(PP:polymer::name->classadditives:substance::class->M),40) replacing a numerical D value
   Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M,40) replacing a numerical D value and setting up Foscale value:
 ADVANCED SYNTAXES (see key2key examples for further details)
  e.g. request based on alternatives
      HDPE|PP:polymer::name->classadditives:substance::class->M
  e.g. request based on superclass defined in "polymerfamily": polyolefin = 'LLDPE;LDPE;MDPE;HDPE;PP'
  polyolefin:polymerfamily::name->polymer:polymer::name->classadditives:substance::class->name:substance::name->M
  e.g. request based on regular expressions (simple regular expressions are accepted)
  \antiUV{3|2}\ :substance::name->M

> fmecaengine is designed to run in paralell (trough several instances) on the computing cluster of JRU 1145
  on either Windows or Linux (preferred for efficiency) nodes.
> Please write, an additional script or function for complex post-treatment. It was not the intend of this script. Please,
  note that for accuracy while preserving memory a linear time scale is used for kinetics and time scale propertional to the
  square root of time is used for concentration profiles.

ADDITIONAL COMMENTS
  Note 1: To add more layers, update the spreadsheet consistently (no need to modify this script/function)
  Note 2: It is expected that simulation chaining is applied to consistent structures (i.e. with a same number of layers)
  Note 3: Any negative Bi value is interpreted as "setoff" simulation (to be placed as a starting node)
  Note 4: Any change in solver paremeters is also detected and forces the whole database to be recaculated
          (use different output folders to store the results from different strategies if required)
  Note 5: For debugging purposes, the structure array s stores all simulation parameters in same order as in the original
          spreadsheet. Use r = senspatankar(senspatankar_wrapper(s(i))) to restart the ith simulation
  Note 6: Creation of PDF files on the fly may interact with antivirus software on windows systems. If you get randomly
          messages such as "print at XXX %temp%\tempfile.ps: Cannot open file: permission denied.", restart the script/function
          and it should solve the issue.

SEE ALSO: FMECASINGLE FMECAROOT BUILDMARKOV KEY2KEY LOADFMECAENGINEDB

DEPENDENCY INFORMATION TO IMPLEMENT THIS SCRIPT/FUNCTION IN OTHER PROJECTS
> Dependencies to other functions (written by INRA\Olivier Vitrac)


DEMO (Fmecaengine v0.25)
        fmecaengine(... without auto expansion
            'local','C:\Data\Olivier\INRA\Etudiants & visiteurs\Audrey Goujon\illustration_fmeca\',...
            'fmecamainfile','illustration_fmecaengine.ods',...
            'inputpath','inputs', ...
            'outputpath','tmp' ...
            );
        fmecaengine(... automatic expansion
            'local','C:\Data\Olivier\INRA\Etudiants & visiteurs\Audrey Goujon\illustration_fmeca\',...
            'fmecamainfile','illustration2_fmecaengine.ods',...
            'inputpath','inputs', ...
            'outputpath','tmp2' ...
            );

DEMO (Fmecaengine v0.27)
        fmecaengine(...
            'local','C:\Data\Olivier\INRA\Etudiants & visiteurs\Audrey Goujon\illustration_fmeca\',...
            'fmecamainfile','illustration3_fmecaengine.ods',...
            'inputpath','inputs', ...
            'outputpath','tmp3' ...
            );

        fmecaengine(...
            'local','C:\Data\Olivier\INRA\Etudiants & visiteurs\Audrey Goujon\illustration_fmeca\',...
            'fmecamainfile','illustration4_fmecaengine.ods',...
            'inputpath','inputs', ...
            'outputpath','tmp4' ...
            );

CONTACT
Any question to this script/function must be addressed to: olivier.vitrac@agroparistech.fr
The script/function was designed to run on the cluster of JRU 1145 Food Process Engineering (admin: Olivier Vitrac)

Migration 2.1 (Fmecaengine v0.45) - 10/04/2011 - INRA\Olivier Vitrac - Audrey Goujon - rev. 26/08/2011
```

See also

argcheck(*), buildmarkov(*), cellcmp(*), dispb, dispf, Dpiringer(*), fileinfo, find_multiple(*), formatfig, formatax, key2key(*), localname, loadods(*), LOADFMECENGINEDB (*), MatchingClosingSymbol, matcmp(*), nearestpoint(*), print_pdf, print_png, rgb, senspatankar(*), senspatankarC(*), setoffpatankar(*), structcmp(*), subplots, wraptext (*) indispensable functions (shared between toolboxes migration and MS) > Commercial tooboxes required: Bioinformatics Toolbox (only for Graph plotting)

key2key

```
key2key returns the values related to keyA:tableA::columnA->tableB::columnB:tableC::columnC->tableD::columnD...
      SCOPE key2key is a multivalued function (in a Mathematical sense) that implements cardinality operations also known as relatio
           between tables via primary key, super key and foreign keys. Implemented relationships include:
           - one-to-one relationships
           - one-to-many relationships
           - many-to-many relationships
           - cascading between keys
          Operations above are applied via an intuitive syntax, different of SQL for concision.
          By default, a UNIQUE operator operator is apply to all relationships involving strings or cell array of strings.
          The request order is respected only for single requests.

   Examples of relationships in connection with FMECAENGINE
       PP:polymer::name->classadditives
       PP:polymer::name->classadditives:substance::class->name
       PP:polymer::name->classadditives:substance::class->M

       Background:
           http://en.wikipedia.org/wiki/Many-to-many_(data_model)
           http://en.wikipedia.org/wiki/Junction_table
           http://en.wikipedia.org/wiki/Foreign_key
           http://en.wikipedia.org/wiki/Superkey
           http://en.wikipedia.org/wiki/Associative_Entities

   Basic syntax: val = key2key(db,key)

      INPUTS
             db: structure such as db.tableX.columnY = numerical value or string
                 alternatively a structure coding for an ODS file such as: db=struct('filename',...,'headers',...)
            key: string or a 1xn/nx1 string cell array coding for
                   keyA:tableA::columnA1->columnA2
                   keyA:tableA::columnA1->columnA2:tableB::columnB1->columnB2
                   keyA:tableA::columnA1->columnA2:tableB::columnB1->columnB2:tableC::columnC1->columnC2
            key can contain be combined with numbers or can contain Matlab expressions (see examples for details)
       NOTE 1: about lists embedded in strings
            db.tableX.columnY and keys can include list of strings.
            Values are separated by symbols: ';' (semi-colon) or  '|' (vertical bar)
            As a rule of thumb, '|' must be preferred in keys as they mimic the behavior or operator OR.
       NOTE 2: about extra spaces
            Spaces are tolerated within key values but note that they are trimmed around ';' and '|'.
            Do not use spaces without checking the reliability of the database content.
       NOTE 3: about regular expressions
            Regular expressions are partly implemented (see the rules below).
            A regular expression must start with symbol '\' and end with '\'
            Symbol '*' must be replaced by '#' (* is reserved for multiplications).
            Symbols '(' and ')' must be replaced by '{' and '}' respectively
            Quantifiers {} must be replaced by {{}}.
            Quantifier ? is available
            Operators | . \d \D \s \W are implemented
            Operators [] ^ $ \< \> (?< (?= (?<! and quantifiers + are not implemented !!!
       NOTE 4: about multiple keys
            When multiple keys are combined in expressions, they must be enclosed within ()
       NOTE 5: about mathematical expressions
           Almost any valid Matlab expressions can be combined with keys.
           Diringer() has been implemented within a syntax simpler than with Matlab conventional one
           Dpiringer(polymercode,key:table1::columnA1->columnB1:table2::columnA2->columnB2 ...->M)
           Dpiringer(polymercode,key:table1::columnA1->columnB1:table2::columnA2->columnB2 ...->M,temperature)

      OUTPUTS
            val: array of values as stored in db when key is a string
                 a nx3 array as [min(values median(values) maximum(values)]

   Advanced syntax: [val,dbout] = key2key(...)
                    dbout: database (loaded if needed)

   Internal syntax: val = key2key(db,key,interpreterflag,recursionflag)
                   interpreterflag (default = true) executes keys as possible Matlab expressions
                   recursionflag (default=false) forces key2key to drop the recursion

   Syntax with specific statistical analysis (works only with cell array of keys)
                    val = key2key(db,keyarray,[],[],percentiles)
                    default percentiles = 5th, 50th, 100th

 TOY EXAMPLES, execute lines between {} with F9 (evaluate)
 %{
  %  EXAMPLE 1 (full toy example)
        key = 'PP:polymer::name->classadditives:substance::class->name';
       db.polymer = ...
           struct('name', {{'LLDPE' 'LLDPE' 'LDPE' 'LDPE' 'MDPE' 'MDPE' 'HDPE' 'HDPE' 'PP' 'PP'}'},...
        'classadditives', {{'antoxidants' 'antiUV' 'antoxidants' 'antiUV' 'antoxidants' 'antiUV' 'antoxidants' 'antiUV' 'antoxidants
                 );
       db.substance = ...
           struct('class', {{'antoxidants' 'antoxidants' 'antoxidants' 'antiUV' 'antiUV' 'antiUV'}'},...
                  'name', {{'antiox1' 'antiox2' 'antiox3' 'antiUV1' 'antiUV2' 'antiUV3'}'},...
                  'M',     [  101       102      103       201       202       203 ]'...
                  );
        key2key(db,key)
 %}
 %{
 %  EXAMPLE 2: Variation based on example 1 (not very useful but illustrate the jump between multiple tables)
        key2 = 'PP:polymer::name->classadditives:substance::class->name:substance::name->M';
        key2key(db,key2)
 %}
 %{
```

```
%  EXAMPLE 3: Variation based on example 2 (use of superclass as key)
    key3 = 'polyolefin:polymerfamily::name->polymer:polymer::name->classadditives:substance::class->name:substance::name->M';
    db.polymerfamily = struct(...
            'name',{{'polyolefin' 'polystyrene'}'},...
            'polymer',{{'LLDPE;LDPE|MDPE;HDPE;PP' 'HIPS;PS'}'} ....
            );
    key2key(db,key3)
%}
%{
%  EXAMPLE 4: Variation based on example 3 (behavior in presence of missing values)
    key4 = 'LDPE|undefined|PP:polymer::name->classadditives:substance::class->name:substance::name->M';
    key2key(db,key4)
%}
%{
%  EXAMPLE 5: Variation based on example 4 (alternative values, note that extra spaces can be included arround operator '|')
    key5 = 'antiUV2 | antiox1 | antiUV3 :substance::name->M';
    key2key(db,key5)
%}
%{
%  EXAMPLES 6: Variation based on example 5 (search all anitUVi with i=0..9)
    key6a = '\antiUV\d\ :substance::name->M';
    key6b = '\antiUV\d{{1}}\ :substance::name->M';
    key6c = '\antiUV\d{{1,1}}\ :substance::name->M';
    key6d = '\antiUV\d?\ :substance::name->M';
    key2key(db,key6a)
    key2key(db,key6b)
    key2key(db,key6c)
    key2key(db,key6d)
%}
%{
%  EXAMPLES 7: Variation based on example 6 (to illustrate the difference beween regular expressions)
    key7a = '\antiUV{3|2}\ :substance::name->M';
    key7b = '\antiUV3|2\ :substance::name->M';
    key7c = '\.#PE.#\:polymer::name->classadditives:substance::class->name:substance::name->M'
    key7d = '\PE\:polymer::name->classadditives:substance::class->name:substance::name->M'
    key7e = 'PE:polymer::name->classadditives:substance::class->name:substance::name->M'
    key2key(db,key7a) % interpreted as containing antiUV3 or containing antiUV2
    key2key(db,key7b) % interpreted as containing antiUV3 or containing 2
    key2key(db,key7c)
    key2key(db,key7d)
    key2key(db,key7e)
%}
%{
%  EXAMPLES 8: with mathematical formula
    key8a = 'Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M)'
    key8b = 'min(Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M,40))';
    key8c = 'Dpiringer(PP,max(PP:polymer::name->classadditives:substance::class->M))'
    key8d = 'min(Dpiringer(PP,PP:polymer::name->classadditives:substance::class->M,100))';
    key8e = 'Dpiringer(LDPE,\antiUV{3|2}\:substance::name->M)';
    key8f = 'Dpiringer(LDPE,[(\antiUV{3|2}\:substance::name->M);(\antiUV1\:substance::name->M)])';
    key2key(db,key8a)
    key2key(db,key8b)
    key2key(db,key8c)
    key2key(db,key8d)
    key2key(db,key8e)
    key2key(db,key8f)
%}
%{
%  EXAMPLE 9: example 8a with double and triple keys
    db.contact = struct('condition',{{'cond1' 'cond2' 'cond3'}},'temperature',[25 40 110]);
    key9a = 'Dpiringer(PP,(PP:polymer::name->classadditives:substance::class->M),(cond3:contact::condition->temperature))';
    key2key(db,key9a)
    db.scenario = struct('id',{{'scenarioA' 'scenarioB' 'scenarioC'}},'polymer',{{'PP' 'LDPE' 'PS'}});
    key9b = 'Dpiringer((scenarioA:scenario::id->polymer),(PP:polymer::name->classadditives:substance::class->M),(cond3:contact::con
    key2key(db,key9b)
    key9c = 'Dpiringer((scenarioA:scenario::id->polymer),(scenarioA:scenario::id->polymer:polymer::name->classadditives:substance::
    key2key(db,key9c)
%}
```

See also

fmecaengine fmecasingle ismemberlist expandtextaslist loadfmecaenginedb

fmecasingle

```
fmecasingle calculate the migration contribution of single steps from FMECA simulations including omitted steps (e.g. Foscale = [0 0])
   SYNTAX  res = fmecasingle(db [,ref,proba])
           [res,resunique] = fmecasingle(...)
   INPUTS
           db: database generated by FMECAENGINE with Foscale=[0 0] forced to all steps
               All considered simulations (possibly independent) must have originally a similar number of steps.
               Simulations can be derived from a previous simulation with modalities (several Foscale or Kscale values possibly combined)
          ref: names or indices of reference steps (by default they are derived from inherit information)
               Reference simulations - simulations before omission/deletion with Foscale - [0 0]
               default = []
        proba: probability of terminal nodes (their sum must be equal to 1)
               It can be an array in the same order as terminal nodes in db
               or a structure such as proba.node = value
               The structure assignment must be preferred when the order is unknown.
               default = [] assigns 1/n where n is the number of terminal nodes

   OUTPUTS
          res: structure with fields coding for all steps used as input (identified from
               res.(step) - [dCF values]
   resunique: multiple structure that match only steps without modalities
               resunique.value.(step0)=[dCF values]
               resunique.id.(step0)={corresponding names}
               resunique.proba.(step0)=[corresponding probabilities]

   Example (used for developement):
       load('C:\Data\Olivier\Communications\LNE2011\drafts\fmecabaseofconditions.mat')
       res = fmecasingle(fmecadb);
       SML=1e-3; severity=@(CF) 100*99./max(100*SML./CF-1,0);
       hfig=figure; formatfig(hfig,'figname','omission_dseverity','paperposition',[ 5.0467    7.2245   10.8907   15.2284]);
       hs = subplots([.2 1],[.6 .4],[],[],'alive',3);
       subplot(hs), hold on, i = 0;
       for step=fieldnames(res)'
           i=i+1;
           res.(step{1}) = struct('dCF',res.(step{1}),'severity',severity(res.(step{1})),'col',interp1(linspace(0,1,64),jet(64),severity(res.(step{1}))'/100 ) );
           res.(step{1}).severity(res.(step{1}).severity==0)=NaN;
           res.(step{1}).col(isnan(res.(step{1}).col))=0;
           plotpub(i*ones(size(res.(step{1})).severity)),res.(step{1}).severity,'markerfacecolor',res.(step{1}).col,'markeredgecolor',res.(step{1}).col,'linestyle','none','markersize',12,'marker','o')
           text(1,0,[step{1} '  '],'fontsize',16,'rotation',90,'HorizontalAlignment','right','VerticalAlignment','middle');
       end
       hr = refline(0,100); set(hr,'color','r','linewidth',2,'linestyle',':');
       hr = refline(0,33); set(hr,'color','c','linewidth',2,'linestyle',':');
       formatax(hs,'fontsize',14,'xticklabel',''), ylabel('Severity','fontsize',16);
       print_png(300,get(gcf,'filename'),'C:\Data\Olivier\Communications\LNE2011\drafts');
```

SEE ALSO

fmecaengine fmecaroot key2key buildmarkov loadfmecaenginedb

fmecaroot

```
fmecaroot returns the root (according to prop) of each node (to be created with FMECAENGINE)
  syntax: root = fmecaroot(fmecadb [,prop])
       fmecadb: output object of FMECAengine
          prop: 'parent' (default) or 'inherit'
```

See also

fmecaengine, fmecasingle, buildmarkov, loadfmecaenginedb, key2key

buildmarkov

```
buildmarkov builds a Markov chain based on a list keywords or values and a list of parent
   [treename,treeind] = buildmarkov(list,parent)
       treename: nx1 cell array giving all possible n paths as names (taken from list)
                 structure generated by fmecaengine
        treeind: nx1 cell array giving all possible n paths as indices
   [treename,treeind,map,succ] = buildmarkov(list,parent,'property',value)
            Implemented properties/values
               sort = 'none' (default), 'ascend' or 'descend'
            map: mxn array (m=max path depth) matching treeind but coded as find_multiple does with format=1
           succ: lxn array (l=max number of children) coding for the list of children (coded as find_multiple does with format=1)

 example
   list =   {'A1' 'B1' 'C1' 'A2' 'A3' 'A4' 'C3' 'C2' 'AA1' 'AA2' 'AB1' 'AB2'}
   parent = {''   ''   ''   'A1' 'A2' 'A3' 'C2' 'C1' 'A1'  'AA1' 'AA1' 'AB1'}
   [pathsnames,pathsind]=buildmarkov(list,parent)
     pathsnames{:}
     ans =
         'A1'    'A2'    'A3'    'A4'
     ans =
         'A1'    'AA1'    'AA2'
     ans =
         'A1'    'AA1'    'AB1'    'AB2'
     ans =
         'B1'
     ans =
         'C1'    'C2'    'C3'
```

SEE ALSO

fmecaengine, fmecasingle, loadfmecaenginedb, key2key, ismemberlist