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Documented models for predicting material, energy and economic balance for all channels,

Acronym: AWAST

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Material, economic, energetic and environmental modelling and simulation tools for the selection, evaluation and optimisation of a complete MSW chain. Contract number: EVK4-CT-2000-00015

> Name of the co-ordinator: Jacques Villeneuve Project home page: <u>http://awast.brgm.fr</u>

Name of the authors: BRGM: Jacques Villeneuve, Pascale Michel, Yannick Ménard TU-Wien/IWA: Roland Fehringer, Bernd Brandt RMA: Hans Daxbeck



Summary

This report is the result of the Work Package 7. It gathers 4 deliverables of the contract:

- D25: Documented models for predicting material and energy balance for all channels, with their methods of use,
- D26: Documented models and databases for economic balance calculation,
- D27: Software allowing the simulation of all possible organisation of solid waste management,
- D28: Methodology, use and limits of the software; report generation options for different types of end-users.

These deliverables have been reorganised in a more coherent document presenting the simulator.

The basic principles of simulation and components of a simulator are presented first. Then follows a detailed description of models that have been included for the different channels: collection/transport, sorting plant, incineration, composting and landfill. All aspects (material, energy, costs) of these models are described together.

The configuration of the simulator allowing to address waste management systems is the object of the report entitled "System definition". It explains how has been designed the general flowsheet of a waste management system as well as the way to represent the different flows of materials in this system.

At last, the methodology to use simulation, including supplied results is presented under the form of a tutorial.



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1. PRESENTATION OF SIMULATION – METHOD AND COMPONENTS OF A SIMULATOR.

1.1. Simulation based approach

In industrial production field, a simulator is basically aimed at helping processing engineers and scientists to model plants operation with available experimental data and to determine optimal treatment configuration that meets production targets. The simulator can also assist plant designers with sizing unit operations required to achieve given circuit objectives.

In Municipal Solid Waste (MSW) management, including treatment of waste, the objectives are a bit more complex:

- get rid-off solid waste (decrease volume, protect public health, eliminate or stabilise toxic elements/substances),
- minimise cost of waste management,
- minimise social and environmental impact/disturbances (employment, participation of citizens, acceptance of treatment plants, medium and long term impacts).

A simulator basically allows to get a representation of a given situation in terms of matter and energy "flows" circulating between "processes". By changing some key parameters of the system (either in input flows or in processes), it calculates the new material and energy balances. It supplies particularly the flows of matter output to the system into the environment. Additionally, the simulator can supply the costs associated to the operations and the "value" of the different flows.

So basically, the simulator does not integrate in itself the interpretation of its results. It remains an advanced calculator containing functions that can manipulate experimental data, calculate coherent material balances, sizes and settings of unit operations, simulate plant operation and display results in tables and graphs.

The simulator combines the following elements (see Figure 1):

The flowsheet describes the system in terms of successive unit operations and material streams. This flowsheet can reflect various scenarii so they can be compared against given criteria. It takes into account numerous system features to describe the physical (sorting plant) as well as functional (sorting of glass) elements.

The phase model describes the materials handled by the system (raw waste, products, reagents, water, etc.) so that unit operations and plant performance, products and reagents quality (grades and undesirable element level) can be evaluated. The phase description is critical for analysing and optimising the system. This statement reinforces the vital importance of field data and sampling protocols.

Mathematical models for each unit operation formalises the current scientific knowledge about the unit operation, and its level of complexity depends on the data available and the targeted objectives (i.e. flowsheeting, unit operation sizing, or optimisation). The model parameters - dimensions, settings and calibration factors - are calculated or validated from field data.

A set of algorithms for data reconciliation, model calibration, unit operation sizing, full material balance calculation, power consumption and costs calculation. These algorithms are interfaced with a set of data representation tools. As a result, the plant simulator constitutes a highly efficient communication vector between the different actors who play a part in the system operation and evolution.





Figure 1: Main functions of a steady-state simulator

1.2. Modelling and reality

The simulation will culminate in the selection and definition of scenarii for the simulator (WP9) "

Unit operation modelling is a way to describe, interpret and try to predict what happens in reality. The modelling task is subject to a series of approximations summarised in Figure 2.



Figure 2. Successive approximations from reality.

The quality of the model strongly depends on each step of approximation.

The first step is "What we can observe from reality". If reality is a composting plant, the collection of data concerning operation of the plant will never provide a complete representation of what really happens. To date, a model built from these data will include this lack of knowledge. On the contrary, if a very precise model was built which necessitates, for example, the gradient of dissolved oxygen concentration in the



neighbourhood of particle surfaces, it is obvious that this data would never be available from any plant to allow the use of this model.

The second step of approximation is "What we can understand from observation". The large number of variables linked to the complexity of phenomena occurring during processing justifies that research has been, and is presently being, carried out in this field on specific subjects. An extensive literature exists on the combustion process, the fermentation and processes less important, but present understanding is still widely based on a "global transfer function approach. This understanding is, of course, a severe approximation. It has the advantages of supplying a means for analysing the material balance in a process, necessitating relatively few experimental data, and taking into account the influence of the previous processes.

The third step of approximation from reality is "What is possible to resolve ?". The resolution of the basic equations describing the physics and chemistry of the system may be difficult or even impossible without hazardous assumptions. Conversely, the difficulty arising from mathematical resolution of equations may lead to the choice of simplified representations of reality.

The last step is "What knowledge is possible to transfer". Any model is a communication tool, and is subject to losses of information when communication occurs. If the knowledge transfer from the model developer to the final user is not properly carried out, the results acquired from use of the model will reflect this loss of information.

As a result of these remarks, the possibility of solving waste management problems using a modelling approach is linked to the extent to which these approximations should be accepted. For preliminary design of a new system, we do not need the same level of precision of simulation results as when trying to increase performance of an existing system by a few percent. It the first case, the results may be evaluated by an experienced process designer whereas in the second case, the results can be compared to plant data and these data can be used to improve the precision of results. The simulator should not offer THE universal mathematical models of processes, but rather a range of methods for data treatment and objective definition, and a range of models allowing different problems to be solved according to the available data and the user's objectives.



2. MODELS OF WASTE TREATMENT PROCESSES

2.1. Collection

The description and methodology of use of the model developed is presented in **annex 1**.

2.2. Transport

11 Distance empty road

13 Frequency (trip/year)

17 Dust emissions (t/year)

12 Distance empty motorway

14 Stock capacity at plant site (t)

15 Type of truck (from database)

16 Emissions of chemical elements (t/year)

Transport - X outputs		17 parameters	X+1 outp	out streams			
#		Parameters		Default value			
1	Number of outputs			Х			
2	Input stream number for	each output		0			
3	Transport by boat, train,	3 (road)					
4	Distance unit (km/trip, kr	1 (km/trip)					
5	Distance loaded urban s		0				
6	Distance loaded urban s		0				
7	Distance loaded road	0					
8	Distance loaded motorw	0					
9	Distance empty urban sl	0					
10	Distance empty urban sl	ow		0			

This model allows calculating the fuel consumption and the total covered distance for the transport of a given material. The number of output streams (X, parameter #1) depends on the number of streams to be transported. Icons with different numbers of outputs are also needed. Outputs number from 1 to X are devoted to materials transport, output number X+1 correspond to the gaseous and dust emissions (off-gas) related to the total covered distance.



Parameters of Equipment #2 Transport - 4 outputs					
Parameters	Values				
Transport definition for each output	Edit				
Transport distances for each output	Edit				
Transport constraints for each output	Edit				
Emissions if known	Edit				

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0

0

0

0

0

0

0

For each output, the input stream number as first to be specified (parameter #2). Transport type (boat, train, road, parameter #3) has also to be defined. Both parameters can be found in the box "Transport definition for each output".

<mark>₩</mark> 8 #2	2 - - Transport - 4 outputs - 1	ransport definition for 📘	
Num	ber of outputs	4	* *
	Input stream number for each output	Transport by	
1	1	road 🔹	
2	2	road 🔹	
3	3	road 🔹	
4	4	road 🚽 🚽	•
		boat train	
		road	

Distance unit (km/trip or km/year) as well as distances for various types of trip can be valued (parameters #4 to #12) for each output.

2 18 #	🖫 #2 Transport - 4 outputs - Transport distances for each output									
Num	Number of outputs 4									
	Distance uni	t	Distance loaded urban slo w	Distance loaded urban fast	Distance loaded road	Distance loaded motorway	Distance empty urban slo w	Distance empty urban fast	Distance empty road	Distance empty motor w ay
1	km/year	-	1000	0	0	0	1000	0	0	0
2	km/trip	-	10	10	0	0	10	10	0	0
3	km/trip	-	10	5	55	0	10	5	55	0
4	km/year	•	100	0	0	2500	100	0	0	2500

Transport model can use constraints (parameters group n°3) to calculate fuel consumption and gaseous emissions. These constraints are:

- frequency (trip/year) (parameter #13),
- stock capacity at plant site (t) (parameter #14),
- type of truck (parameter #15).

28 #2	🎘 #2 Transport - 4 outputs - Transport constraints for each output							
Num	ber of outputs	4						
	Frequency (trips/year)	Stock capacity at plant site (t)	Type of truck (from database)					
1	0	0	0					
2	120	0	1					
3	70	0	2					
4	0	10000	0					

Eventually, the user can value the parameters #16 and #17 which correspond to the total production (gaseous + particles) of exhaust fumes.

##2 Transport - 4 outputs - Emissions of chemical elements (t/year)										
Number of out	Number of outputs									
Phases	ias AWAS1									
Composition	02	H20	CO org.	CO fossil	CO2 org.	CO2 fossil	CH4	NO2	SO2	F2
1	0	0	0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0	
3	0	0	0	0	0	0	0	0	0	
4	0	0	0	0	0	0	0	0	0	

Calculation flowchart is described hereafter.







The only necessary data to run this model is the transport distance, either in km/year or km/trip. The model structure allows to use known data but if nothing else than the distance is known, it calculates the energy consumption and emissions for all possible transport means

All basic data concerning fuel type, consumption and emissions from the different types of trucks are in a database stored in file "Messages.txt" and can be modified and adjusted.

2.3. Sorting plants

Sorting - X outputs	8 parameters	X+1 output streams
---------------------	--------------	--------------------

#	Parameters	Default value
1	Number of outputs	Х
2	Split of feed (%)	0
3	Nominal capacity (tons/year)	0
4	Number of sorting lines	1
5	Mechanisation level (low, medium, high, very high)	1
6	Capital cost (euros)	0
7	Process investment (euros/year)	0
8	Building investment (euros/year)	0

The model can be use for different type of sorting plant with a different number of sorted products. The $X_{.}$ first outputs correspond to the sorted materials and the sorting residues, the last one (X+1) stands for the off-gas stream.



This model uses a split matrix (box "transfer coefficient", parameter #2) of the different categories of the waste feed to calculate the composition of each output streams.

Parameters of Equipment #1 Sorting - 3 outputs				
Parameters	Values			
Transfer coefficients	Edit			
Sorting cost calculation	Edit			

🗱 #1 Sorting - 3 outputs - Transfer coefficients									<u>- 0 ×</u>
number of outp	put			* *					
Phases	aste AWAS								
Composition	Wood	Paper	Glass	Fe Metals	NFe Metals	Plastics	Textiles	Biowaste	Others
Composition 1	Wood 0	Paper 90	Glass O	Fe Metals O	NFe Metals O	Plastics 0	Textiles O	Biowaste O	Others O
Composition 1 2	Wood 0 0	Paper 90 0	Glass O O	Fe Metals 0	NFe Metals O O	Plastics 0 80	Textiles 0 0	Biowaste O O	Others 0 0
Composition 1 2 3	Wood 0 0 100	Paper 90 0 10	Glass 0 0 100	Fe Metals 0 0 100	NFe Metals 0 0 100	Plastics 0 80 20	Textiles 0 0 100	Biowaste 0 0 100	Others 0 0 100

The second box holds the necessary parameters for cost calculation. The capital cost can be valued through parameter #6 if it is known. Otherwise, it is calculated from the



nominal capacity of the plant (parameter #3), the number of sorting lines (parameter #4) and the mechanisation level (parameter #5). Operating costs include direct, indirect, repair and renewal costs. Process and building investments can be valued for more accurate cost assessments. Default cost calculation uses the effective waste flow entering the plant and the sorting plant database (in file Messages.txt) which can be easily modified and updated. The assessment of the capital cost (CC) and the operating costs (OC) allows the assessment of the production cost (PC) according to:

PC = CC / LF + OC,

where LF stands for the lifespan of the sorting plant.

###1 Sorting - 3 outputs - Sorting cost calculation	
Parameters	Values
Nominal capacity (if 0, calculated), tons/year	10000
Number of sorting lines	2
Mechanization level	high 🔻
Capital cost (if 0, default calculation), euros/year	0
Process investment (if 0, default calculation), euros/year	0
Building investment (if 0 default calculation), euros/year	0

2.4. Incineration

Two models have been produced.

2.4.1. Level (0) incineration

	Incinerator 10 parameters One output		One output stream
#		Parameters	Default value
1	% of chemical element in	n bottom ash	0
2	% of chemical element in	n fly ash	0
3	% of waste mass in botto	om ash	17
4	% of waste mass in fly ash		2
5	Category used for bottom and fly ash		0
6	Component used for flue gas		0
7	Regulation (yes or no)		Yes
8	Calculated air flowrate (N	Nm3/h)	0
9	Excess oxygen ratio		1
10	Coefficients for regulatio	n calculation	0

This model uses a split matrix of the different chemical elements of the waste feed to calculate the chemical composition of the bottom ash, fly ash and flue gas output streams of an incineration plant (including furnace and flue gas treatment). Fly ash contains as well fly ash recovered from the boiler and the filter and the filter cake produced during the treatment of the flue gas cleaning water. Flue gas stream corresponds to the stack output.





Incinerator (0)

The phase model needs to contain at least

- one waste phase described in terms of categories and user-defined sub-populations giving the chemical composition of the different categories,
- one gas phase used for combustion air and flue gas description. It contains a userdefined sub-population description giving the chemical composition of the gas with exactly the same chemical elements in the same order than the chemical elements of the waste phase.

Parameters of Equipment #1 Incinerator (0)	
Parameters	Values
% of chemical element in ash	Edit
% of waste mass in ash	Edit
Category used for bottom and fly ash	Edit
Component used for flue gas	Edit
Combustion air regulation	Edit

The interface for parameter input is divided in different groups:

The first group gives the percentage of the different waste chemical elements going to the bottom (parameter #1) and fly (parameter #2) ash:



1 🕫 🗱 🕂 🗧 🕅	nerator (0) - %	of chemical element i	in ash 📃 🗖 🗙
Phases	User defined ub-population 1	% of chemical element in bottom ash	% of chemical element in fly ash
Waste AWAS	0	0	0
	Ή	0	0
	C	1.4	0.7
	N	0	0
	S	33.4	49
	CI	9.1	55.94
	F	61.8	31.78
	Р	86.3	13.75
	Fe	98.7	1.284
	AI	0	0
	РЬ	67.2	32.349
	Zn	56.8	43.717
	Cd	20.1	77.912
	Hg	3.7	62
	Remainder	0	0

The remaining part (100% - % in bottom ash - % in fly ash) reports to the flue gas stream.

This split matrix concerns the critical chemical elements for which data are available. Concerning the chemical elements not appearing in the list (grouped in "Remainder"), it is necessary to have a global mass transfer from the waste feed to the bottom (parameter #3) and fly (parameter #4) ash output streams, giving by the second group of parameters:

🎇 #1 - 🛛 Incinerator (0) - % of waste mass i 📃 🗖 🗙				
Phases	% of waste mass in bottom ash	% of waste mass in fly ash		
Waste AWAS	17	2		

The remaining part (100% - % in bottom ash - % in fly ash) reports to the flue gas stream.

The "Remainder" split coefficients are calculated to reach this global split coefficients.

Bottom and fly ash are described using the waste phase. The parameter #5 gives the typical composition of ash in terms of waste categories:

👷 🛙 🕂 🗧 🕅	nerator (0) - Ca	ategory u 📃 🗖 🗙
Phases	Composition	Category used for bottom and fly ash
Waste AWAS	Wood	0
	Paper	0
	Glass	0
	Fe-metals	0
	Non Fe-metal:	0
	Plastic	0
	Textiles	0
	Food waste	0
	Water	0
	Others	100



The mass of ash generally reports to a category receiving this kind of waste.

If the gas phase contains different components (molecular components), it is necessary to indicate which component will receive the mass of flue gas generated during combustion. The parameter #6 gives this typical composition.

Air regulation

The last group concerns the combustion air regulation:

## #1 - Incinerator (0) - Combustion air regulation	_ 0	×
Parameters	Values	
Regulation	yes	•
Calculated air flowrate (Nm3/h)		0
Excess oxygen ratio		1
Coefficients for regulation calculation	Edit	

If the parameter #7 is "Yes", the feedrate of combustion air is calculated keeping the composition of the input gas. This calculated value is written in the output parameter #8. The necessary air flowrate is calculated by taking into account the excess oxygen ratio (parameter #9 which is 1 for stoichiometric proportion and greater than 1 for excess) and the mass stoichiometric coefficients for oxygen consumption (parameter #10).

These coefficients take into account the typical air composition - 23.1% in weight of oxygen in the following example:

🍽 #1 - 🗉 Incinerator (0) - Coefficient 📃 🗖 🗙		
Phases	User defined ub-population 1	Coefficients for regulation calculation
Waste AWAS	0	-4.33
	'н	34.64
	C	11.5467
	N	0
	S	4.33
	CI	0
	F	0
	Р	0
	Fe	0
	AI	0
	РЬ	0
	Zn	0
	Cd	0
	Hg	0
	Remainder	0

2.4.2. Level (3) incineration.

Floduced steall	67 parameters	Three output streams Bottom ash Flue gas Produced steam
		67 parameters

#	Parameters	Default value
1	Process (Furnace, Furnace+boiler or Furnace+TAG)	Furnace+TA



		G
2	Stream number of combustion air	0
3	Stream number of feed water	0
4	Phase number of waste (unused)	0
5	Unburned percentage of waste categories	0
6	Reactive percentage of chemical elements per waste category	100
7	Reactive percentage of components for other phases	1
8	Numbers of reaction	0
9	Chemical reaction numbers	0
10	Chemical reaction levels	1
11	Chemical reaction ratios	100
12	Typical ash composition	0
13	Ash percentage giving flying ash	1
14	Combustion air regulation (No, Total combustion or Flue gas O2)	No
15	Oxygen set-point in flue gas	0
16	Energy calculated parameters (Efficiency or Temperature)	Efficiency
17	A	0
18	В	0
19	C	0
20	D	0
21	Global efficiency of the incinerator (electric yield)	0
22	Efficiency of the furnace/boiler/TAG (thermal yield)	0
23	Efficiency of the TAG	0
24	Efficiency of the boiler/heat exchanger	0
25	Temperature of flue gas in heat-exchanger/boiler entry (°C)	800
26	Pressure of flue gas in heat-exchanger/boiler entry (bar)	1
27	Enthalpy of flue gas in heat-exchanger/boiler entry (kW)	0
28	Exergy of flue gas in heat-exchanger/boiler entry (kW)	0
29	Temperature of flue gas in heat-exchanger/boiler output (°C)	200
30	Pressure of flue gas in heat-exchanger/boiler output (bar)	1
31	Enthalpy of flue gas in heat-exchanger/boiler output (kW)	0
32	Exergy of flue gas in heat-exchanger/boiler output (kW)	0
33	Temperature of water in heat-exchanger/boiler entry (°C)	20
34	Pressure of water in heat-exchanger/boiler entry (bar)	1
35	Enthalpy of water in heat-exchanger/boiler entry (kW)	0
36	Exergy of water in heat-exchanger/boiler entry (kW)	0
37	Temperature of steam in heat-exchanger/boiler output (°C)	350
38	Pressure of steam in heat-exchanger/boiler output (bar)	35
39	Enthalpy of steam in heat-exchanger/boiler output (kW)	0
40	Exergy of steam in heat-exchanger/boiler output (kW)	0
41	I emperature of steam in turbine output (°C)	100
42	Pressure of steam in turbine output (bar)	1.2
43	Enthalple of steam in turbine output (KW)	0
44	Exergy of steam in turbine output (KW)	0
45	Temperature of the boiler (°C)	150
46	Pressure of the Doller (Dar)	40
4/	Enthalpy of water in the boiler (KVV)	0
48	Exergy of water in the boiler (KVV)	0
49	Entimalpy of steam in the beiler (KW)	0
50	Exergy of Steam in the poller (KVV)	0
51	Liteouric energy (KVV)	0
52	Latent neal (KJ/Ky) Nominal canacity (tons / year)	0
55	Information about number of workers (no or yes)	U No
-04	(10001 40001 1000000 0) = 0000000000000000000000	INU



55	Number of worker per socio-professional category 1	1
56	Number of worker per socio-professional category 2	1
57	Number of worker per socio-professional category 3	1
58	Factor of capital cost (euros / ton)	1
59	Constant of capital cost (euros)	1
60	Factor of worker cost (euros / ton)	1
61	Constant of worker cost (keuros)	1
62	Factor of fixed cost	1
63	Electricity purchase cost (euros / kWh)	1
64	Maintenance cost per quantity of incinerated waste (euros / ton)	1
65	Factor of repairs and renewal cost	1
66	Electricity selling price (euros / kWh)	1
67	Fixed bonus linked to the sell of energy	1
68	Flue gas treatment system (dry / semi-wet / wet)	dry
69	Stream number of feed water used for flue gas treatment	0
70	Stream number of feed reagents used for flue gas treatment	0

This model simulates a furnace with energy recovery.

Depending on the value of the parameter #1, the model can take into account:

- Only the furnace with calculation of mass transfer during combustion from the waste feed to the bottom ash and flue gas (including fly ash) outputs.
- Furnace + heat exchanger/boiler where the combustion energy is converted into steam energy throw the heat exchanger/boiler device. The steam circuit (input and output) is used for the water flowrate and can take place into a heating circuit.
- Furnace + heat exchanger/boiler + turbine/alternator group (TAG) where the steam energy is converted into mechanical energy through the turbine then in electrical energy through the alternator. The residual steam energy can be used into an heating circuit.

The model has three outputs: bottom ash, flue gas with fly ash and produced steam, and at least three inputs: fuel (Municipal Solid Waste), combustion air and water (or steam) to feed the steam circuit:

Furnace + Heat exchanger/boiler + Turbo-alternator group



An optional water input can be added to take into account process water used for temperature regulation in the combustion chamber.



The internal structure of the model can be summarised by the following scheme:



Parameter groups

Due to the great number of parameters, the input interface uses different parameter groups:

Parameters of Equipment #1 - Furnace Turbine-alternator grou - Inc	cinerator (3)	
Parameters	Values	
Process	Furnace+TA	.G 🔻
Stream number of combustion air		1
Stream number of feed water		1
Unburned percentage of waste categories	Edit	
Reactive percentage of chemical elements per waste category	Edit	
Reactive percentage of components for other phases	Edit	
Chemical reactions	Edit	
Typical ash composition	Edit	
Ash percentage giving flying ash		1
Combustion air regulation	No	-
Component set-point in flue gas	Edit	
Energetic balance	Edit	
Calorific capacity parameters	Edit	
Cost calculation	Edit	

The parameters #2 and #3 gives the stream number as displayed on the flowsheet for the combustion air feed and the steam circuit input respectively.

The parameters from "Unburned percentage of waste categories" to "Ash percentage giving flying ash" describe the mass transfer as a set of chemical reactions.

The parameters "Combustion air regulation" and "Component set-point in flue gas" determine how to calculate the quantity of combustion air.

The "Energetic balance" and "Calorific capacity parameters" groups are devoted to the energetic balance calculation.

The last group concerns the capital, operating and production costs calculation.



Phase model requirement and use

Furnace is considered as a chemical reactor where waste is burned with air to produce bottom ash, gas and fly ash. Sometimes water is injected into the furnace to regulate the gas temperature.

Feed waste stream is described using the waste phase.

The waste phase is divided into different categories. Each category is defined by its chemical content (especially C, O, H, N, S, Cl, F, heavy metals...) using a sub-population description.

C can be described using 2 sub-populations: C fossil (fossil carbon) and C org (organic carbon) to be able to characterize the CO_2 production.

Sometime moisture is included in the different categories, otherwise it is identified as a water phase. The two cases are taken into account.

Bottom ash stream is described using the waste phase: the unburned part of each category remains into the category itself, ash produced during combustion of burned part reports to a special category into the finer size class.

Flue gas and fly ash stream is described using the waste phase for the fly ash and the gas phase for produced gas. Fly ash is limited to a special category into the finer size class.

Combustion air stream is described using the gas phase with the standard air composition.

Process water stream, if it exists, is described using the water phase.

Material transformation

The following scheme summarizes the transformation of one category of waste during the combustion stage.



Each category is divided into a burned part and an unburned part. The unburned part remains into the category itself and goes with bottom ash. The unburned percentage of each category is given by the parameter #5.

Each chemical element of the burned part is divided into a reactive part available for the chemical reactions and a non-reactive part, which reports directly to ash. The



percentage of the reactive part of each chemical element of each category is given by the parameter #6.

Similarly, the gas (or other phase) components are divided into a reactive and a non-reactive part with the percentage given by the parameter #7.

Each chemical element of each category will react with other elements or air components following chemical reactions:

 $\begin{array}{l} 2O \rightarrow O_2 \\ 2C \text{ fossil} + O_2 \rightarrow 2CO \text{ fossil} \\ 2C \text{ org} + O_2 \rightarrow 2CO \text{ org} \\ 2CO \text{ fossil} + O_2 \rightarrow 2CO_2 \text{ fossil} \\ 2CO \text{ org} + O_2 \rightarrow 2CO_2 \text{ org} \\ 4H + O_2 \rightarrow 2H_2O \text{ (gas)} \end{array}$

The following interface allows to select the different chemical reactions (parameter #9) occurring during combustion and to sort them in different levels (parameter #10) with different ratios (parameter #11):

11 B	🏽 🕮 #1 Incinerator (3) - Chemical reactions					
Num	bers of reaction		10	_ :		
	Chemical reaction numbe	ers	Chemical reaction levels	Chemical reaction ratios		
1	Water vapour	•	1	100		
2	02 production	•	1	100		
3	N2 production	•	1	100		
4	C -> CO org.	•	2	100		
5	CO -> CO2 org.	•	3	100		
6	C -> CO fossil	•	4	100		
7	CO -> CO2 fossil	•	5	100		
8	H2O production	•	6	100		
9	NO2 fuel production	•	7	100		
10	NO2 gas production	•	8	100		

These reactions are limited using the reactive part as described above.

Ash produced from the burned parts of all the categories reports to a specific category corresponding to the waste classification of ash. This category is chosen using the parameter #12:

🅦 #1 - 🗉 Incinerator (3) - Typical ash 📃 🗖 🗙			
Phases	Composition	Typical ash composition	
Waste AWAS	Putrescible	0	
	Papers	0	
	Cardboards	0	
Composites		0	
Textiles		0	
Health care te		0	
Plastics		0	
Unclas. Comb		0	
	Glass	0	
	Metals	0	
Unclas. Unco		100	
Special MSW		0	
	Fines	0	

Ash is divided into a small part as fly ash and the remaining part as bottom ash as indicated by the parameter #13 (Ash percentage giving flying ash).



Combustion air

The quantity of combustion air can be calculated:

- To be just in excess for total combustion.
- To respect a flue gas component content.

The parameter #14 indicates if the quantity of combustion air is calculated or not and what is the objective of the regulation. The parameter #15 gives the component content in flue gas if the regulation is calculated using this objective.

Mass balance equations

 Q_{ij} Partial flowrate of chemical element (sub-population) j of category i of waste phase

 Q_j Partial flowrate of chemical element j: $Q_j = \sum_i Q_{ij}$

 Q_i Partial flowrate of category i: $Q_i = \sum_i Q_{ij}$

 q_{pi} Partial flowrate of component i of phase p: $q_{pi} = Q_i$ if p is the waste phase

 U_i Unburned percentage of the category i (parameter #5)

 r_{ij} Reactive percentage of chemical element j in category i of the waste phase for the burned part (parameter #6)

 r_{pi} Reactive percentage of component i of phase p (parameter #7)

 X_i Percentage of ash going into the category i (parameter #12)

 α Ash percentage in flying ash (parameter #13)

 R_{pi} Partial flowrate of component i of the phase p which will participate to the chemical reaction. In the case of waste phase the component corresponds to the chemical element.

$$R_{pj} = \sum_{i} Q_{ij} \frac{100 - U_i}{100} \frac{r_{ij}}{100}$$
 if p is the waste phase

$$R_{pi} = q_{pi} \frac{r_{pi}}{100}$$
 otherwise

After solving of the chemical reaction system

 P_{ni} Products (containing remaining reagents)

Bottom ash stream

Partial flowrate of chemical element j of category i in waste phase

$$Q_{ij}\frac{U_i}{100} + \frac{X_i}{100}\frac{100 - \alpha}{100} \left(P_{pj} + \sum_k Q_{kj}\frac{100 - U_k}{100}\frac{100 - r_{kj}}{100}\right) \text{ where } p \text{ is the waste}$$

phase

Partial flowrate of component i in water phase

$$q_{pi} \frac{100 - r_{pi}}{100} + P_{pi}$$
 where p is the water phase



Flue gas and flying ash stream

Partial flowrate of chemical element j of category i in waste phase (for flying ash)

$$\frac{X_i}{100} \frac{\alpha}{100} \left(P_{pj} + \sum_i Q_{ij} \frac{100 - U_i}{100} \frac{100 - r_{ij}}{100} \right)$$
 where p is the waste phase

Partial flowrate of component i in gas phase

$$q_{pi} \frac{100 - r_{pi}}{100} + P_{pi}$$
 where p is the gas phase

Energetic balance

The following interface groups together the parameters for energetic balance:

📲 #1 - Furnace Turbine-alternator grou - Incinerator (3) - Energetic balance 🔰 🔲 🗙			
Parameters	Values		
Temperature of combustion air (*C)	25		
Energy calculated parameters	Efficiency 👻		
Global efficiency of the incinerator (electric yield)	0.220711		
Efficiency of the furnace/boiler (thermal yield)	0.799881		
Efficiency of the TAG	0.94593		
Efficiency of the boiler	0.917562		
Temperature of flue gas in heat-exchanger/boiler entry (*C)	1020		
Pressure of flue gas in heat-exchanger/boiler entry (bar)	1		
Enthalpy of flue gas in heat-exchanger/boiler entry (kW)	26652.6		
Exergy of flue gas in heat-exchanger/boiler entry (kW)	15086.5		
Temperature of flue gas in heat-exchanger/boiler output (*C)	220		
Pressure of flue gas in heat-exchanger/boiler output (bar)	1		
Enthalpy of flue gas in heat-exchanger/boiler output (kW)	5224.88		
Exergy of flue gas in heat-exchanger/boiler output (kW)	1121.79		
Temperature of water in heat-exchanger/boiler entry (*C)	150		
Pressure of water in heat-exchanger/boiler entry (bar)	36		
Enthalpy of water in heat-exchanger/boiler entry (kW)	5375		
Exergy of water in heat-exchanger/boiler entry (kW)	777.103		
Temperature of steam in heat-exchanger/boiler output (*C)	380		
Pressure of steam in heat-exchanger/boiler output (bar)	30		
Enthalpy of steam in heat-exchanger/boiler output (kW)	26474.7		
Exergy of steam in heat-exchanger/boiler output (kW)	8280.33		
Temperature of steam in turbine output (*C)	110		
Pressure of steam in turbine output (bar)	1		
Enthalpie of steam in turbine output (kW)	22034.6		
Exergy of steam in turbine output (kW)	2564.02		
Temperature of the boiler (*C)	214.034		
Pressure of the boiler (bar)	35		
Enthalpy of water in the boiler (kW)	7669.55		
Exergy of water in the boiler (kW)	1591.41		
Enthalpy of steam in the boiler (kW)	9107.96		
Exergy of steam in the boiler (kW)	1303.38		
Electric energy (kW)	4200		

In the heat-exchanger/boiler the water is vaporized, and it exits as a saturated steam. The energy necessary to change water properties is given by the flue gas. The thermodynamic steam energy is transformed in mechanical energy in the turbine then in electrical energy by the alternator.

The energy balance is calculated using the thermodynamic variables: enthalpy (H_i), entropy (S_i) and exergy (Ex_i - where i refers to the number of the stream as displayed with the internal structure scheme). The general expression of exergy is: $Ex_i = H_i - T_{ref}S_i$



where T_{ref} is the temperature of the reference status.

The energy balance can be calculated following two different ways:

- The temperatures are known and the efficiencies are calculated
- The efficiencies of the different stages are known and the temperatures are back-calculated.

The parameter #16 gives the chosen way.

The efficiencies are known and the temperatures are calculated

The global efficiency of the incinerator (parameter #21) and the waste energy give the produced electric energy (output parameter #51 in kW):

$$W_e = \eta_{\text{incinerator}} W_w$$

The waste energy is given by the mean Low Heating Value and the flowrate of the waste:

$$W_w = \sum_i Q_i LHV_i$$

where LHV_i is the low heating value of the waste category i.

Knowing the TAG efficiency (parameter #23) one obtains the enthalpy variation of steam through the turbine:

$$\Delta H_{\rm TAG} = H_5 - H_4 = -\frac{W_e}{\eta_{\rm TAG}}$$

The enthalpy variation of steam through the heat exchanger/boiler is linked to the efficiency of the furnace/boiler set (or thermal yield - parameter #22) by:

$$\Delta \boldsymbol{H}_{\mathrm{HEB}} = \boldsymbol{H}_{4} - \boldsymbol{H}_{7} + \boldsymbol{H}_{6} - \boldsymbol{H}_{3} = \boldsymbol{\eta}_{\mathrm{thermal}} \boldsymbol{W}_{\mathrm{W}}$$

where H_6 and H_7 refer to the enthalpy of liquid water and the enthalpy of steam in the boiler respectively.

The enthalpy variation of the flue gas crossing the heat exchanger/boiler is the opposite of the previous variation taking into account the efficiency of the heat exchanger/boiler (parameter #24):

$$\Delta H_{\rm flue\,gas} = H_2 - H_1 = -\frac{\Delta H_{\rm HEB}}{\eta_{\rm HEB}}$$

Enthalpies and entropies are function of the temperature and the pressure as they are linked to the calorific capacity of the different components of the flue gas or of the steam.

The calorific capacity is expressed as a polynomial function of the temperature:

$$c_p = AT^3 + BT^2 + CT + D$$

where the coefficients A, B, C and D are given by the parameters #17, #18, #19 and #20 respectively for the different components of flue gas.

The latent heat for phase change is also an important parameter for the calculation of thermodynamic properties. The parameter #52 gives the latent heat for the different components of the flue gas (essentially for water component).

These five parameters are initialized in the "Calorific capacity parameters" group:



Phases Composition A B C Gas AWAST 02 -1.88E-012 -1.19E-007 H20 -2.39E-010 7.03E-007 CO org. 0 0	0.000408 3.91E-005 0	D 0.8021 1.7956	Latent heat (kJ/kg) 0
Gas AWAST 02 -1.88E-012 -1.19E-007 H20 -2.39E-010 7.03E-007 C0 org. 0 0 0	0.000408 3.91E-005 0	0.8021 1.7956	0
H20 -2.39E-010 7.03E-007 C0 org. 0 0	3.91E-005 0	1.7956	0400 74
CO org. 0	0		2496.71
		0	0
CO fossil 0 0	0	0	0
CO2 org. 2.2E-010 -9.21E-007	0.00144	0.4923	0
CO2 fossil 2.2E-010 -9.21E-007	0.00144	0.4923	0
CH4 0 0	0	0	0
NO2 0 0	0	0	0
S02 0 0	0	0	0
F2 0 0	0	0	0
Cl2 0 0	0	0	0
HCI 0 0	0	0	0
Cd 0 0	0	0	0
Hg O O	0	0	0
N2 -1.66E-010 4.37E-007	-0.000155	1.0486	0

The enthalpy (output parameter #27), the entropy and the exergy (output parameter #28) of the flue gas after combustion and before heat exchanger can be calculated as its temperature (parameter #25) and its pressure (parameter #26) are known:

$$H_1 = H(T_1, P_1)$$

$$S_1 = S(T_1, P_1)$$

The enthalpy (H_2 - output parameter #31) of the flue gas after heat exchanger/boiler can then be calculated. Its temperature (output parameter #29) can be deducted knowing the pressure (parameter #30). The entropy and the exergy (output parameter #32) are then calculated.

The enthalpy (output parameter #35), the entropy and the exergy (output parameter #36) of the feed water in the steam circuit can be calculated as its temperature (parameter #33) and its pressure (parameter #34) are known:

$$H_3 = H(T_3, P_3)$$
 $S_3 = S(T_3, P_3)$

From the known boiler pressure (parameter #46) the boiler temperature (output parameter #45) is calculated using the expression:

$$T_6 = A_b P_6^3 + B_b P_6^2 + C_b P_6 + D_b$$

The enthalpy (H_6 - output parameter #47), the entropy and the exergy (output parameter #48) of the water in the boiler, as well as the enthalpy (H_7 - output parameter #49), the entropy and the exergy (output parameter #50) of the steam in the boiler, can be calculated using the latent heat:

$$L_{\nu} = A_l P_6^4 + B_l P_6^3 + C_l P_6^2 + D_l P_6 + E_l$$

The enthalpy (H_4 - output parameter #39) of the steam after heat exchanger/boiler can then be calculated. Its temperature (output parameter #37) can be deducted knowing the pressure (parameter #38). The entropy and the exergy (output parameter #40) are then calculated.

Knowing H_4 , the enthalpy of the steam in turbine output (H_5 - output parameter #43) is deducted as well as the temperature (output parameter #41), knowing the pressure (parameter #42), the entropy and the exergy (output parameter #44).

The temperatures are known and the efficiencies are calculated

Using equations displayed above, the enthalpies, entropies and exergies of the different streams are calculated and the enthalpy variations are deducted.

Knowing the waste energy and the produced electric energy, it is possible to obtain the different efficiencies (output parameters #21-24).



All the thermodynamic variables measured or calculated by the model are summarized and displayed into the "Operating Parameters" and "Calculated Power Consumption" files.

Capital and operating costs calculation

📲 #1 incinérateur - Cost calculation	
Parameters	Values
Nominal capacity (tons / year)	0
Information about number of workers	yes 👻
Number of worker per socio-professional category 1	3
Number of worker per socio-professional category 2	5
Number of worker per socio-professional category 3	15
Factor of capital cost (euros/ton)	275.8
Constant of capital cost (euros)	1.82315E+007
Factor of worker cost (euros/ton)	5.85
Constant of worker cost (keuros)	256.3
Factor of fixed cost	1.43
Electricity purchase cost (euros/kWh)	0.0442
Maintenance cost per quantity of incinerated waste (euros/ton)	1.5
Factor of repairs and renewal cost	0.02
Electric selling price to the electric producer (euros/kWh)	0.0042
Fixed bonus linked to the sell of energy	0
Flue gas treatment system	semi-wet 👻
Stream number of water used for flue gas treatment	0
Stream number of reagents used for flue gas treatment	0

The model calculates the capital cost (CC) related to the building of an incinerator, the rated capacity of which is given by the parameter #53. If parameter #53 is set to 0, the model uses the waste stream mass flow rate together with parameters #58 and #59.

Operating costs (OP) calculation takes into account fixed costs (FC), relative costs (RC), repairs and renewal costs (RRC) and energy income (EI).

- Fixed cost is usually composed of very heterogeneous charges. In most cases, the wage bill stands for approximately 75 % of these costs. According to the value of parameter #54, the model performs automatic calculation or not. If the number of worker in each socio-professional category is known (parameters #55, #56 and #57), the model then uses default value for salaries. If not, fixed costs are calculated with parameters #59 and #60 through a proportional relation between the wage bill and the capacity of the incinerator.
- Reagents charges stand for more than half the relative costs. If parameter #69 (stream of reagents used for the whole cleaning gas process) and parameter #70 (stream of water used for the whole cleaning gas process) are valued then reagents and water charges are calculated using the corresponding information (mass flow rate of each constituent) together with prices given in tab 1. Otherwise, they are calculated with default values of specific mass flow rate listed in tab. 1. Electricity (parameter #63) consumption depends on the flue gas treatment system (see tab1). Electricity and Maintenance (parameter #64) charges add to the amount.
- Repairs and renewal cost calculation is carried out from parameter #65 through a linear relation with the capital cost.
- Only one type of income is considered: it is related to the sale of electricity (with parameter #66) calculated from the electricity produced in the case of the presence of a turbo alternator group. A fixed bonus linked to the sell of energy can be valued. If it is not, the corresponding income is null. The income linked to the recuperation and the sale of metals is not taken into account since it most often appears negligible in front of energy income.

Operating costs are then evaluated according to:



OP = FC + RC + RRC - EI.Production costs (PC) take into account the lifespan (LF) of the plant: PC = CC / LF + OP + EI

Economical data are listed in a configuration file of the software (messages.txt) and can be easily modified to precisely represent the economical reality of a given country.

			Process type		
		Dry	Semi-wet	Wet	
		Quantities	, kg/t of inciner	ated waste	Price, euros/t of reagents
Water (m3	8/t)	0	0.3	1	0.152
Lime		17	17	6	92
Bicarbona	te of soda	22	*	*	190
Soda		*	*	2	230
Activated of	carbon	1	1	1	610
Coke		2.5	2.5	2.5	610
Ammonio	SNCR	10	10	10	150
Ammonia	SCR	5	5	5	150
		Electricity	y consumption, icinerated was	kWh/t of te	
		70	80	85	

Tab 1: Quantities and prices of water and reagents used for flue gas treatment

2.5. Composting plant

Incinerator	10 parameters	Two output stream

#	Parameters	Default value
1	Unaltered part of waste categories (%)	0
2	Reactive percentage of waste elements per waste categories	100
3	Reactive percentage of all other elements	100
4	Number of reactions	0
5	Chemical reaction numbers	0
6	Chemical reaction levels	1
7	Chemical reaction ratios	100
8	Compost distribution in each category (%)	0
9	Process type (Windrows, Rotating drum, Enclosed halls)	1
10	Nominal capacity (tons/year)	0

This model simulates the fermentation stage of a composting plant. It has two outputs: a gaseous stream corresponding to the off-gas emitted during the fermentation (drying, carbon dioxide and ammonia production, etc.) and a solid stream for the production of compost.





The input interface uses different parameters group:

Parameters of Equipment #1 Composting				
Parameters	Values			
Unaltered part of waste categories (%)	Edit			
Reactive percentage of waste elements per waste category	Edit			
Reactive percentage of all other elements	Edit			
Chemical reactions	Edit			
Compost distribution in each category (%)	Edit			
Cost calculation	Edit			

The parameters from "unaltered part of waste categories" to "Compost distribution in each categories describe the mass transfers between phases and waste categories.

The last group is devoted to cost assessments.

The fermentation process is considered as a chemical reactor where waste is biologically transformed to produce off-gas and compost. Feed waste stream is described using the waste phase. The waste phase is divided into different categories. Each category is defined by its chemical content (especially C, O, H, N, S, Cl, F, heavy metals...) using a sub-population description. Carbon content can be described using 2 sub-populations: C fossil (fossil carbon) and C org (organic carbon) to be able to characterize the CO_2 production.

Each category is divided into a reacting part and an unaltered part. The unaltered part remains into the category itself and goes with compost. The unaltered percentage of each category is given by the parameter #1.

💥 #7 - Composting park - Composting 💻 🗖 🗙				
Phases	Composition	Unaltered part of waste categories (%)		
Waste AWAS	Wood	63.3		
	Paper	45		
Glass		44.6		
Fe Metals		100		
	NFe Metals	30.3		
	Plastics	56.2		
Textiles		56.1		
Biowaste		15.1		
	Others	100		

The percentage of the reactive part of each chemical element of each category is given by the parameter #2

In the same way, the gas and liquid components are divided into a reactive and a nonreactive part according to the percentage given by the parameter #3.



😹 #7 - Composting park - Composting - Reactive percentage of waste elements per waste category 📃 🗐 🗙							
Waste AWAST							
	Н	Cfossil	Corg	N	0	S	
Wood	90	0	90	90	90	0	
Paper	80	0	80	80	80	0	
Glass	0	0	0	0	0	0	
Fe Metals	0	0	0	0	0	0	
NFe Metals	0	0	0	0	0	0	
Plastics	5	5	5	5	5	0	
Textiles	5	5	5	5	5	0	
Biowaste	95	0	95	95	95	0	
Others	25	25	25	25	25	0	
•						Þ	

Chemical reactions, defined in phase model, can be selected through the following interface (parameter #5), sorted in different levels (parameter #6) with different ratios (parameter #7).

₩ 8 #1	📲 #7 - Composting park - Composting - Chemical reactions 📃 🔲 🗙					
Number of reactions						
	Chemical reaction number	ers	Chemical reaction levels	Chemical reaction ratios		
1	H -> H2O	•	1	100		
2	Corg -> CO2org	•	2	100		
3	N -> NH3	•	3	100		
4	0 -> 02	•	4	100		
5	water -> H2O vap	•	5	100		

The total number of reactions is given by the parameter #4. These reactions are limited by the reactive and unaltered part given by parameter #2 and parameter #3.

Compost produced from the reactive part of all categories, can be distributed into each category through parameter #8.

🎇 #7 - Composting park - Composting 💻 🔲 🗙		
Phases	Composition	Compost distribution in each category (%)
Waste AWAS	Wood	0
	Paper	0
	Glass	15
	Fe Metals	1.5
	NFe Metals	0
	Plastics	4
	Textiles	0
	Biowaste	1.5
	Others	78

The last two parameters are dedicated to cost assessments. Parameter #9 allows to specify the process type (Windrows, Rotating drum, Enclosed halls), parameter #10 gives the nominal capacity (tons/year) of the composting plant used for capital cost assessment. Operating costs are calculated from the effective waste flowrate entering the composting plant. All other data used for costs assessments are in file "Messages.txt" and can be modified and adjusted.



🎇 #7 - Composting park - Composting - Cost calculation	
Parameters	Values
Process type	Windrows 🔹
Nominal capacity (tons/year)	40000

2.6. Landfill

The description of the model in presented in annex 2 as a final report.



3. SYSTEM DEFINITION

"This section deals with the definition of an adequate system for the project AWAST. Basis for the system are project objectives and MFA methodology. The first part is dedicated to the definition of the system boundary, then follow definitions of the investigated types of waste and the design of the system structure. The next step covers definitions of processes and goods and illustrates links between processes and between work packages. Finally the selection of substances and the waste matrix complete the system definition."

Please refer to the report in annex 3 entitled " Deliverables 25, 26, 27, 28, System Definition – AWAST".



4. ANNEXES

- 4.1. Annex 1: Collection/transport models
- 4.2. Annex 2: Landfill models
- 4.3. Annex 3: System definition AWAST
- 4.4. Annex 4: System definition Figures
- 4.5. Annex 5: System definition Waste matrices

