# Materials & Streams Report for SimV2

### 1. OVERALL PROCESS DATA

Annual Operating Time	7,872.38 h
Unit Production Ref. Rate	8,288.27 kg MP/yr
Batch Size	104.91 kg MP
Recipe Batch Time	99.65 h
Recipe Cycle Time	99.65 h
Number of Batches per Year	79.00

MP = Flow of Component 'Pheromone' in Stream 'PHERO'

# 2.1 STARTING MATERIAL REQUIREMENTS (per Section)

Section	Starting Material	Active Product	Amount Needed (kg Sin/kg MP)	Molar Yield (%)	Mass Yield (%)	Gross Mass Yield (%)
Main Section	(none)	(none)	0.00	Unknown	Unknown	Unknown

Sin = Section Starting Material, Aout = Section Active Product

# 2.2 BULK MATERIALS (Entire Process)

Material	kg/yr	kg/batch	kg/kg MP
AHM	5,530	70.00	0.67
Biomass	8	0.10	0.00
Ethyl Acetate	40,829	516.82	4.93
Glucose	3,786	47.93	0.46
NaCl	8	0.10	0.00
Peptone	2,840	35.95	0.34
Prenol	7,900	100.00	0.95
Water	183,584	2,323.85	22.15
TOTAL	244,485	3,094.75	29.50

# 2.3 BULK MATERIALS (per Section)

#### **SECTIONS IN: Main Branch**

Main Section			
Material	kg/yr	kg/batch	kg/kg MP
AHM	5,530	70.00	0.67
Biomass	8	0.10	0.00
Ethyl Acetate	40,829	516.82	4.93
Glucose	3,786	47.93	0.46
NaCl	8	0.10	0.00
Peptone	2,840	35.95	0.34
Prenol	7,900	100.00	0.95
Water	183,584	2,323.85	22.15
TOTAL	244,485	3,094.75	29.50

# 2.4 BULK MATERIALS: SECTION TOTALS (kg/kg MP)

Raw Material	Main Section
AHM	0.67
Biomass	0.00
Ethyl Acetate	4.93
Glucose	0.46
NaCl	0.00
Peptone	0.34
Prenol	0.95
Water	22.15
TOTAL	29.50

# 2.5 BULK MATERIALS: SECTION TOTALS (kg/batch)

Raw Material	Main Section
AHM	70.00
Biomass	0.10
Ethyl Acetate	516.82
Glucose	47.93
NaCl	0.10
Peptone	35.95
Prenol	100.00
Water	2,323.85
TOTAL	3,094.75

# 2.6 BULK MATERIALS: SECTION TOTALS (kg/yr)

Raw Material	Main Section
AHM	5,530
Biomass	8
Ethyl Acetate	40,829
Glucose	3,786
NaCl	8
Peptone	2,840
Prenol	7,900
Water	183,584
TOTAL	244,485

# 2.7 BULK MATERIALS (per Material)

AHM				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-14	100.00	5,530	70.00	0.67
TOTAL	100.00	5,530	70.00	0.67
Biomass				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-1	33.33	3	0.03	0.00
P-4	33.33	3	0.03	0.00
P-7	33.33	3	0.03	0.00
TOTAL	100.00	8	0.10	0.00

Ethyl Acetate				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-12	86.46	35,299	446.82	4.26
P-14	13.54	5,530	70.00	0.67
TOTAL	100.00	40,829	516.82	4.93
Glucose				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-16	100.00	3,786	47.93	0.46
TOTAL	100.00	3,786	47.93	0.46
NaCl				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-11	100.00	8	0.10	0.00
TOTAL	100.00	8	0.10	0.00
Peptone				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-16	100.00	2,840	35.95	0.34
TOTAL	100.00	2,840	35.95	0.34
Prenol				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-11	100.00	7,900	100.00	0.95
TOTAL	100.00	7,900	100.00	0.95
Water				
Procedure	% Total	kg/yr	kg/batch	kg/kg MP
Main Section (Main Branch)				
P-1	0.02	35	0.45	0.00
P-4	0.02	35	0.45	0.00
P-7	0.02	35	0.45	0.00
P-11	0.43	782	9.90	0.09
P-16 TOTAL	99.52 100.00	182,697 183,584	2,312.61 2,323.85	22.04 22.15
17.11.0.1		4 OO EO A	0 000 05	22.45

## 3. STREAM DETAILS

Stream Name	Media	S-125	S-126	S-105
Source	INPUT	P-16	P-15	P-15
Destination	P-16	P-15	P-1	P-4
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	35.00	35.00	35.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	998.54	994.89	994.89	994.89
Total Enthalpy (kW-h)	68.11	95.35	31.79	31.78
Specific Enthalpy (kcal/kg)	24.45	34.24	34.24	34.24
Heat Capacity (kcal/kg-°C)	0.98	0.98	0.98	0.98
Component Flowrates (kg/batch)				
Glucose	47.93	47.93	15.98	15.98
Peptone	35.95	35.95	11.98	11.98
Water	2,312.61	2,312.61	771.03	770.79
TOTAL (kg/batch)	2,396.49	2,396.49	798.99	798.75
TOTAL (L/batch)	2,400.00	2,408.81	803.10	802.85

Stream Name	S-112	S-113	GAS03	S-115
Source	P-15	INPUT	P-7	P-7
Destination	P-7	P-7	OUTPUT	P-9
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	35.00	25.00	37.00	25.00
Pressure (bar)	1.01	1.01	1.01	0.96
Density (g/L)	994.89	998.38	1.63	995.96
Total Enthalpy (kW-h)	31.78	0.01	0.09	22.67
Specific Enthalpy (kcal/kg)	34.24	24.96	7.59	24.68
Heat Capacity (kcal/kg-°C)	0.98	1.00	0.21	0.99
Component Flowrates (kg/batch)				
Acetic-Acid	0.00	0.00	0.00	1.78
Biomass	0.00	0.03	0.00	5.36
Carb. Dioxide	0.00	0.00	8.58	0.00
Glucose	15.98	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.88	0.00
Oxygen	0.00	0.00	0.27	0.00
Peptone	11.98	0.00	0.00	11.98
Water	770.79	0.45	0.00	771.24
TOTAL (kg/batch)	798.75	0.48	9.72	790.35
TOTAL (L/batch)	802.85	0.48	5,969.62	793.56

Stream Name	S-116	S-117	WASTE03	S-106
Source	P-9	P-8	P-8	INPUT
Destination	P-8	P-10	OUTPUT	P-4
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	18.00	30.00	30.00	25.00
Pressure (bar)	0.96	0.96	0.96	1.01
Density (g/L)	998.47	993.82	1,001.83	998.38
Total Enthalpy (kW-h)	16.25	26.02	1.07	0.01
Specific Enthalpy (kcal/kg)	17.69	29.61	26.79	24.96
Heat Capacity (kcal/kg-°C)	0.98	0.99	0.89	1.00
Component Flowrates (kg/batch)				
Acetic-Acid	1.78	1.71	0.07	0.00
Biomass	0.00	0.00	0.00	0.03
Cell Debris	5.14	0.00	5.14	0.00
Kinase 2	0.21	0.21	0.01	0.00
Peptone	11.98	11.53	0.45	0.00
Water	771.24	742.49	28.75	0.45
TOTAL (kg/batch)	790.35	755.94	34.41	0.48
TOTAL (L/batch)	791.57	760.65	34.35	0.48

Stream Name	GAS02	S-108	S-109	S-110
Source	P-4	P-4	P-6	P-5
Destination	OUTPUT	P-6	P-5	P-10
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	37.00	25.00	18.00	30.00
Pressure (bar)	1.01	0.96	0.96	0.96
Density (g/L)	1.63	995.96	998.47	993.82
Total Enthalpy (kW-h)	0.09	22.67	16.25	26.02
Specific Enthalpy (kcal/kg)	7.59	24.68	17.69	29.61
Heat Capacity (kcal/kg-°C)	0.21	0.99	0.98	0.99
Component Flowrates (kg/batch)				
Acetic-Acid	0.00	1.78	1.78	1.71
Biomass	0.00	5.36	0.00	0.00
Carb. Dioxide	8.58	0.00	0.00	0.00
Cell Debris	0.00	0.00	5.14	0.00
Kinase 1	0.00	0.00	0.21	0.21
Nitrogen	0.88	0.00	0.00	0.00
Oxygen	0.27	0.00	0.00	0.00
Peptone	0.00	11.98	11.98	11.53
Water	0.00	771.24	771.24	742.49
TOTAL (kg/batch)	9.72	790.35	790.35	755.94
TOTAL (L/batch)	5,969.62	793.56	791.57	760.65

Stream Name	WASTE02	Biomasa	GAS01	S-101
Source	P-5	INPUT	P-1	P-1
Destination	OUTPUT	P-1	OUTPUT	P-3
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	30.00	25.00	37.00	25.00
Pressure (bar)	0.96	1.01	1.01	0.96
Density (g/L)	1,001.83	998.38	1.63	995.96
Total Enthalpy (kW-h)	1.07	0.01	0.09	22.68
Specific Enthalpy (kcal/kg)	26.79	24.96	7.59	24.68
Heat Capacity (kcal/kg-°C)	0.89	1.00	0.21	0.99
Component Flowrates (kg/batch)				
Acetic-Acid	0.07	0.00	0.00	1.78
Biomass	0.00	0.03	0.00	5.36
Carb. Dioxide	0.00	0.00	8.58	0.00
Cell Debris	5.14	0.00	0.00	0.00
Kinase 1	0.01	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.88	0.00
Oxygen	0.00	0.00	0.27	0.00
Peptone	0.45	0.00	0.00	11.98
Water	28.75	0.45	0.00	771.47
TOTAL (kg/batch)	34.41	0.48	9.72	790.59
TOTAL (L/batch)	34.35	0.48	5,971.41	793.80

Stream Name	S-102	S-103	WASTE01	S-121
Source	P-3	P-2	P-2	P-10
Destination	P-2	P-10	OUTPUT	P-11
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	18.00	30.00	30.00	30.00
Pressure (bar)	0.96	0.96	0.96	0.96
Density (g/L)	998.47	993.82	1,001.83	993.82
Total Enthalpy (kW-h)	16.26	26.03	1.07	78.06
Specific Enthalpy (kcal/kg)	17.69	29.61	26.79	29.61
Heat Capacity (kcal/kg-°C)	0.98	0.99	0.89	0.99
Component Flowrates (kg/batch)				
Acetic-Acid	1.78	1.71	0.07	5.13
Biomass	0.00	0.00	0.00	0.00
CDS	0.21	0.21	0.01	0.21
Cell Debris	5.15	0.00	5.15	0.00
Kinase 1	0.00	0.00	0.00	0.21
Kinase 2	0.00	0.00	0.00	0.21
Peptone	11.98	11.54	0.45	34.61
Water	771.47	742.72	28.75	2,227.70
TOTAL (kg/batch)	790.59	756.17	34.42	2,268.06
TOTAL (L/batch)	791.81	760.87	34.36	2,282.17

Stream Name	Prenol	Buffer	S-119	S-122
Source	INPUT	INPUT	P-11	INPUT
Destination	P-11	P-11	P-12	P-12
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	25.00	25.00	25.00
Pressure (bar)	1.01	1.01	9.32	1.01
Density (g/L)	804.50	999.56	993.56	893.64
Total Enthalpy (kW-h)	1.89	0.29	67.02	5.90
Specific Enthalpy (kcal/kg)	16.22	24.86	24.25	11.35
Heat Capacity (kcal/kg-°C)	0.65	0.99	0.97	0.45
Component Flowrates (kg/batch)				
Acetic-Acid	0.00	0.00	5.13	0.00
CDS	0.00	0.00	0.21	0.00
Chrysanthemol	0.00	0.00	90.07	0.00
Ethyl Acetate	0.00	0.00	0.00	446.82
Kinase 1	0.00	0.00	0.21	0.00
Kinase 2	0.00	0.00	0.21	0.00
NaCl	0.00	0.10	0.10	0.00
Peptone	0.00	0.00	34.61	0.00
Prenol	100.00	0.00	10.00	0.00
Water	0.00	9.90	2,237.60	0.00
TOTAL (kg/batch)	100.00	10.00	2,378.13	446.82
TOTAL (L/batch)	124.30	10.00	2,393.55	500.00

Stream Name	EXT	REF	ET-AC	S-120
Source	P-12	P-12	P-13	P-13
Destination	P-13	OUTPUT	OUTPUT	P-14
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	25.00	77.22	196.69
Pressure (bar)	2.00	2.00	1.01	1.01
Density (g/L)	904.87	994.56	832.08	824.60
Total Enthalpy (kW-h)	7.33	65.59	18.05	11.70
Specific Enthalpy (kcal/kg)	11.83	24.63	35.08	111.27
Heat Capacity (kcal/kg-°C)	0.47	0.99	0.45	0.57
Component Flowrates (kg/batch)				
Acetic-Acid	0.00	5.13	0.00	0.00
CDS	0.00	0.21	0.00	0.00
Chrysanthemol	86.47	3.60	0.43	86.04
Ethyl Acetate	446.82	0.00	442.35	4.47
Kinase 1	0.00	0.21	0.00	0.00
Kinase 2	0.00	0.21	0.00	0.00
NaCl	0.00	0.10	0.00	0.00
Peptone	0.00	34.61	0.00	0.00
Prenol	0.00	10.00	0.00	0.00
Water	0.00	2,237.60	0.00	0.00
TOTAL (kg/batch)	533.29	2,291.66	442.79	90.51
TOTAL (L/batch)	589.36	2,304.19	532.15	109.76

Stream Name	AHM	S-123	S-124	DIST
Source	INPUT	INPUT	P-14	P-17
Destination	P-14	P-14	P-17	OUTPUT
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	25.00	20.00	101.18
Pressure (bar)	1.01	1.01	8.14	1.01
Density (g/L)	994.70	893.64	978.25	854.00
Total Enthalpy (kW-h)	0.23	0.92	2.31	8.00
Specific Enthalpy (kcal/kg)	2.82	11.35	8.63	55.69
Heat Capacity (kcal/kg-°C)	0.11	0.45	0.43	0.55
Component Flowrates (kg/batch)				
AAM	0.00	0.00	7.95	7.79
AHM	70.00	0.00	7.00	6.93
Chrysanthemol	0.00	0.00	32.15	30.54
Ethyl Acetate	0.00	70.00	39.81	39.81
Ethyl Alcohol	0.00	0.00	18.12	18.12
Pheromone	0.00	0.00	104.93	0.01
Water	0.00	0.00	20.47	20.47
TOTAL (kg/batch)	70.00	70.00	230.43	123.67
TOTAL (L/batch)	70.37	78.33	235.55	144.82
Stream Name	PHERO			
Source	P-17			
Destination	OUTPUT			
Stream Properties				
Activity (U/ml)	0.00			
Temperature (°C)	393.45			
Pressure (bar)	1.01			
Density (g/L)	832.13			
Total Enthalpy (kW-h)	14.37			
Specific Enthalpy (kcal/kg)	115.80			
Heat Capacity (kcal/kg-°C)	0.29			
Component Flowrates (kg/batch)				
AAM	0.16			
AHM	0.07			
Chrysanthemol	1.61			
Ethyl Acetate	0.00			
Pheromone	104.91			
TOTAL (kg/batch)	106.76			
TOTAL (L/batch)	128.29			

# 4. OVERALL COMPONENT BALANCE (kg/batch)

COMPONENT	INITIAL	INPUT	OUTPUT	FINAL	IN-OUT
AAM	0.00	0.00	7.95	0.00	- 7.95
Acetic-Acid	0.00	0.00	5.33	0.00	- 5.33
AHM	0.00	70.00	7.00	0.00	63.00
Biomass	0.00	0.10	0.00	0.00	0.10
Carb. Dioxide	0.00	0.00	25.73	0.89	- 26.63
CDS	0.00	0.00	0.21	0.00	- 0.21
Cell Debris	0.00	0.00	15.43	0.00	- 15.43
Chrysanthemol	0.00	0.00	36.18	0.00	- 36.18
Ethyl Acetate	0.00	516.82	482.17	0.00	34.65
Ethyl Alcohol	0.00	0.00	18.12	0.00	- 18.12
Glucose	0.00	47.93	0.00	0.00	47.93
Kinase 1	0.00	0.00	0.21	0.00	- 0.21
Kinase 2	0.00	0.00	0.21	0.00	- 0.21
NaCl	0.00	0.10	0.10	0.00	0.00
Nitrogen	5.40	0.00	2.63	2.76	0.00
Oxygen	1.64	0.00	0.80	0.84	0.00
Peptone	0.00	35.95	35.95	0.00	0.00
Pheromone	0.00	0.00	104.93	0.00	- 104.93
Prenol	0.00	100.00	10.00	0.00	90.00
Water	0.00	2,323.85	2,344.32	0.00	- 20.47
TOTAL	7.04	3,094.75	3,097.28	4.50	0.00
				Overall Error:	0,000%

#### **5. EQUIPMENT CONTENTS**

FR-101				
Procedure	Operation	Time (in h)	Volume (in L)	Vapor (in kg)
P-1	START	0.00	0.00	1.18
P-1	TRANSFER-IN-1 (Transfer In)	33.58	803.09	1.18
P-1	CHARGE-2 (Charge)	81.83	803.57	1.18
P-1	HEAT-1 (Batch Heating)	81.92	803.58	1.18
P-1	FERMENT-1 (Batch Kinetic Fermentation)	97.92	797.25	0.34(*)
P-1	COOL-1 (Batch Cooling)	98.40	793.80	0.34(*)
P-1	TRANSFER-OUT-1 (Transfer Out)	99.65	0.00	0.34(*)

<sup>(\*)</sup> Contains material in vapor phase other than Oxygen & Nitrogen

FR-102				
Procedure	Operation	Time (in h)	Volume (in L)	Vapor (in kg)
P-4	START	0.00	0.00	1.18
P-4	TRANSFER-IN-1 (Transfer In)	33.58	802.85	1.18
P-4	CHARGE-2 (Charge)	81.83	803.33	1.18
P-4	HEAT-1 (Batch Heating)	81.92	803.34	1.18
P-4	FERMENT-1 (Batch Kinetic Fermentation)	97.92	797.01	0.34(*)
P-4	COOL-1 (Batch Cooling)	98.40	793.56	0.34(*)
P-4	TRANSFER-OUT-1 (Transfer Out)	99.65	0.00	0.34(*)

<sup>(\*)</sup> Contains material in vapor phase other than Oxygen & Nitrogen

FR-103				
Procedure	Operation	Time (in h)	Volume (in L)	Vapor (in kg)
P-7	START	0.00	0.00	1.18
P-7	TRANSFER-IN-1 (Transfer In)	33.58	802.85	1.18
P-7	CHARGE-2 (Charge)	81.83	803.33	1.18
P-7	HEAT-1 (Batch Heating)	81.92	803.34	1.18
P-7	FERMENT-1 (Batch Kinetic Fermentation)	97.92	797.01	0.34(*)
P-7	COOL-1 (Batch Cooling)	98.40	793.56	0.34(*)
P-7	TRANSFER-OUT-1 (Transfer Out)	99.65	0.00	0.34(*)

<sup>(\*)</sup> Contains material in vapor phase other than Oxygen & Nitrogen

R-101				
Procedure	Operation	Time (in h)	Volume (in L)	Vapor (in kg)
P-11	START	0.00	0.00	3.17
P-11	TRANSFER-IN-1 (Transfer In)	1.25	2,282.17	3.17
P-11	CHARGE-1 (Charge)	0.42	2,407.00	3.17
P-11	CHARGE-2 (Charge)	0.27	2,416.99	3.17
P-11	COOL-1 (Batch Cooling)	0.51	2,407.54	3.17
P-11	REACT-1 (Batch Stoich. Reaction)	1.00	2,393.55	3.17
P-11	TRANSFER-OUT-1 (Transfer Out)	2.25	0.00	3.17

R-102				
Procedure	Operation	Time (in h)	Volume (in L)	Vapor (in kg)
P-14	START	0.00	0.00	0.32
P-14	TRANSFER-IN-1 (Transfer In)	0.40	102.60	4.78(*)
P-14	CHARGE-1 (Charge)	1.25	99.76	69.86(*)
P-14	CHARGE-2 (Charge)	1.25	198.14	46.86(*)
P-14	COOL-1 (Batch Cooling)	1.04	241.58	0.32
P-14	REACT-1 (Batch Stoich. Reaction)	1.00	235.55	0.32
P-14	TRANSFER-OUT-1 (Transfer Out)	2.25	0.00	0.32

<sup>(\*)</sup> Contains material in vapor phase other than Oxygen & Nitrogen