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APMF 2016

# Eco-industrial park design and operation

## Modelling, Optimisation, and System Integration


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CAM.CREATE C4T Cambridge Centre for Carbon Reduction in Chemical Technology

# Outline

1. Introduction
2. Modelling and optimisation for eco-industrial parks
3. System integration for eco-industrial parks
4. Conclusions and future works


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# 1. Introduction



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# 1.1 Industrial ecology

## ➢ Industry

- Resources are harvested and processed for a wide range of value-adding purposes
- Products are ultimately disposed of, recycled or reprocessed
- Despite a significant increase in waste materials recovery, the end of the life cycle for most products is still disposal

## ➢ Ecology

- In natural systems, there is little or no waste
- Organisms produce waste which becomes the products used in a continuous production and consumption system as it passes along the biological food and reproduction chain

## ➢ Industrial ecology

- Mimic the efficiencies of natural and biological systems
- Utilise the emission and waste flows of industry and consumption
- Minimise waste by applying a disposal system for industry via an ecological framework
- Recycle and exchange by-product materials in a sustainable manner


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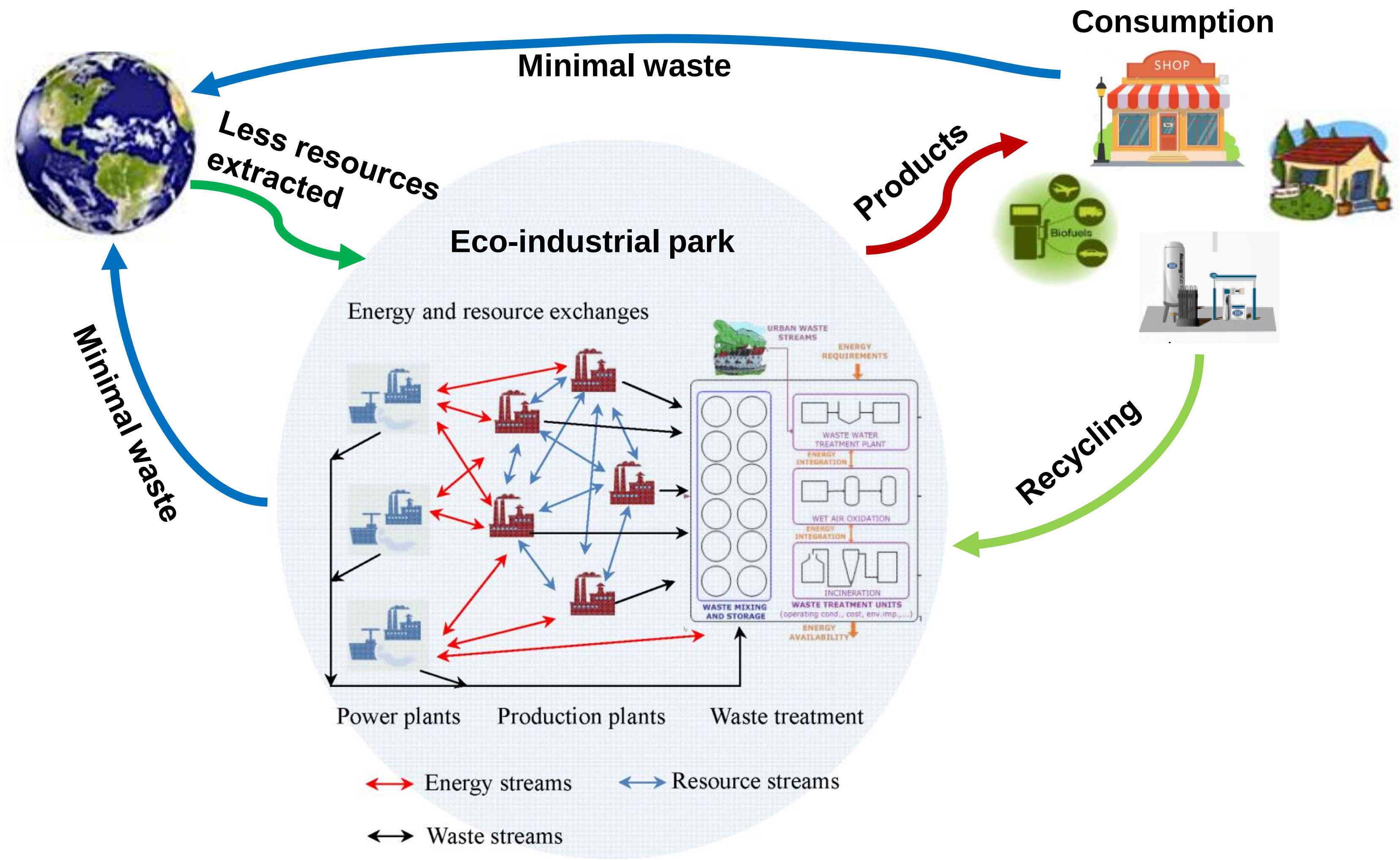
# 1.2 Eco-industrial park





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# 1.3 Eco-industrial park (methodologies)

| | Traditional work | Our work |
|---|---|---|
| **Methods** | • Life Cycle Analysis (LCA)<br>• Network Analysis<br>• Exergy Analysis | • Hierarchy modelling<br>• Advanced mathematical modelling<br>• Optimisation<br>• System integration |
| **Objectives** | • Understand the interactive processes within an existing industrial park (the management of energy and resource flows between each sector)<br>• Evaluate the efficiency of resource utilization and the environmental potential effect<br>• Figure out the sectors affecting the system significantly<br>• Provide suggestions of improving the whole system performance | • An industrial park is described as a four-level hierarchy system from bottom to top: unit operations, to processes, plants and industrial networks<br>• The operations at each industrial park level can be modelled and optimised by using advanced mathematical modelling and optimisation approaches<br>• A smart system (industry 4.0): the industrial park can be displayed, monitored, simulated, and optimised on a system integration platform |
| **Advantages/ disadvantages** | Provide general suggestions (rather than detailed technical supports) to improve resource and energy efficiency for industrial parks | Goes down to each industrial park's component level, thus can provide detailed information for the whole park optimisation |



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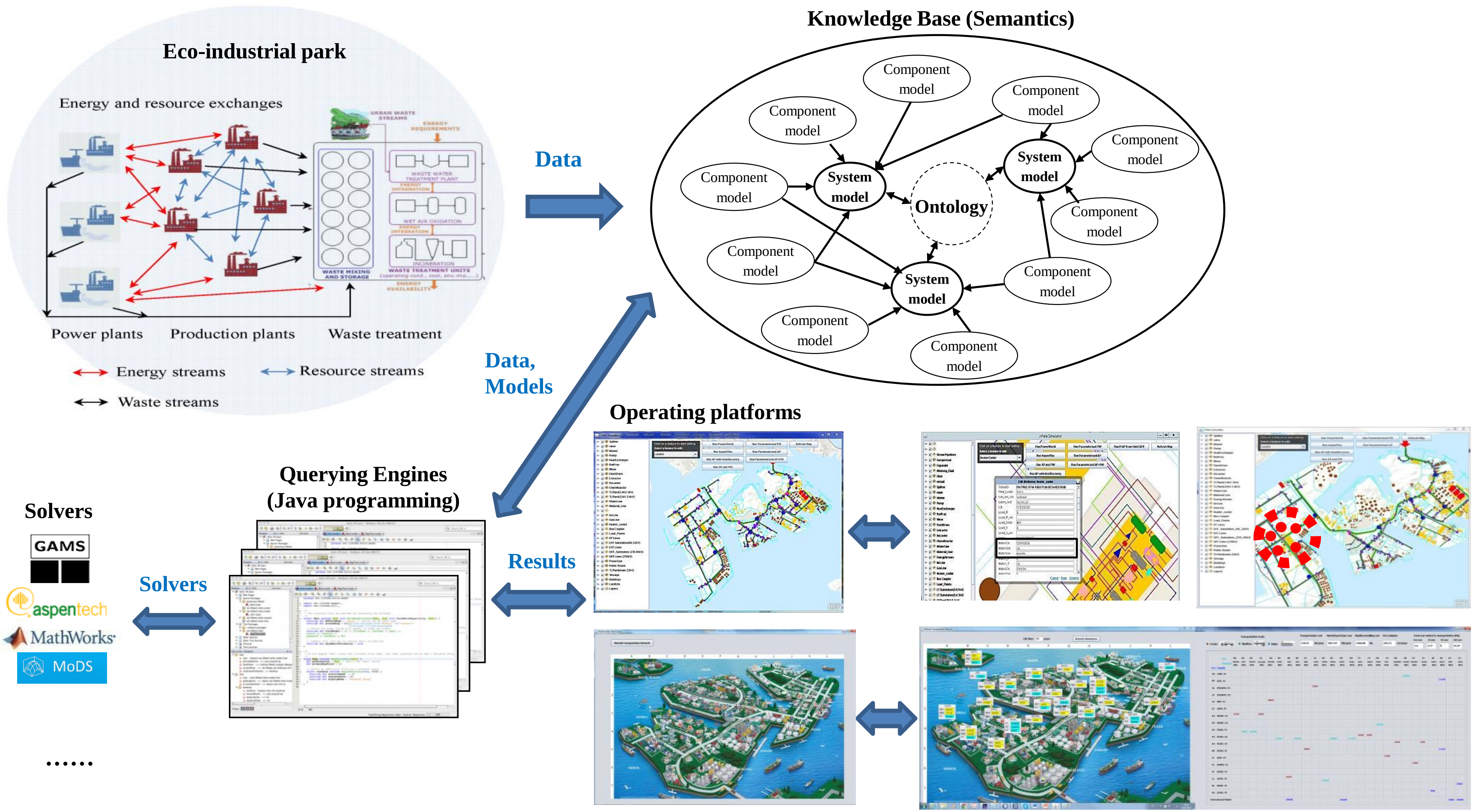
# 1.4 Eco-industrial park (our work: system integration)



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# 1.4 Eco-industrial park (our work)

## Challenges

- **Complex industrial systems composed of a large number of components (units, processes and plants)**

  Multi-level modelling, hierarchy models

- **Detailed operations and performances of industrial systems and the relevant components (units, processes and plants)**

  Advanced modelling methods, surrogate models

- **Optimisation of industrial systems, and optimal operations of industrial components**

  Novel optimisation approaches for solving large scale Mixed Integer Non-linear Programming (MINLP) problems and Mixed Integer linear Programming (MILP) problems

- **System integration and software development for the smart industrial park**

  Semantics, Query, Java programming


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# 2. Modelling and optimisation methods for eco-industrial parks


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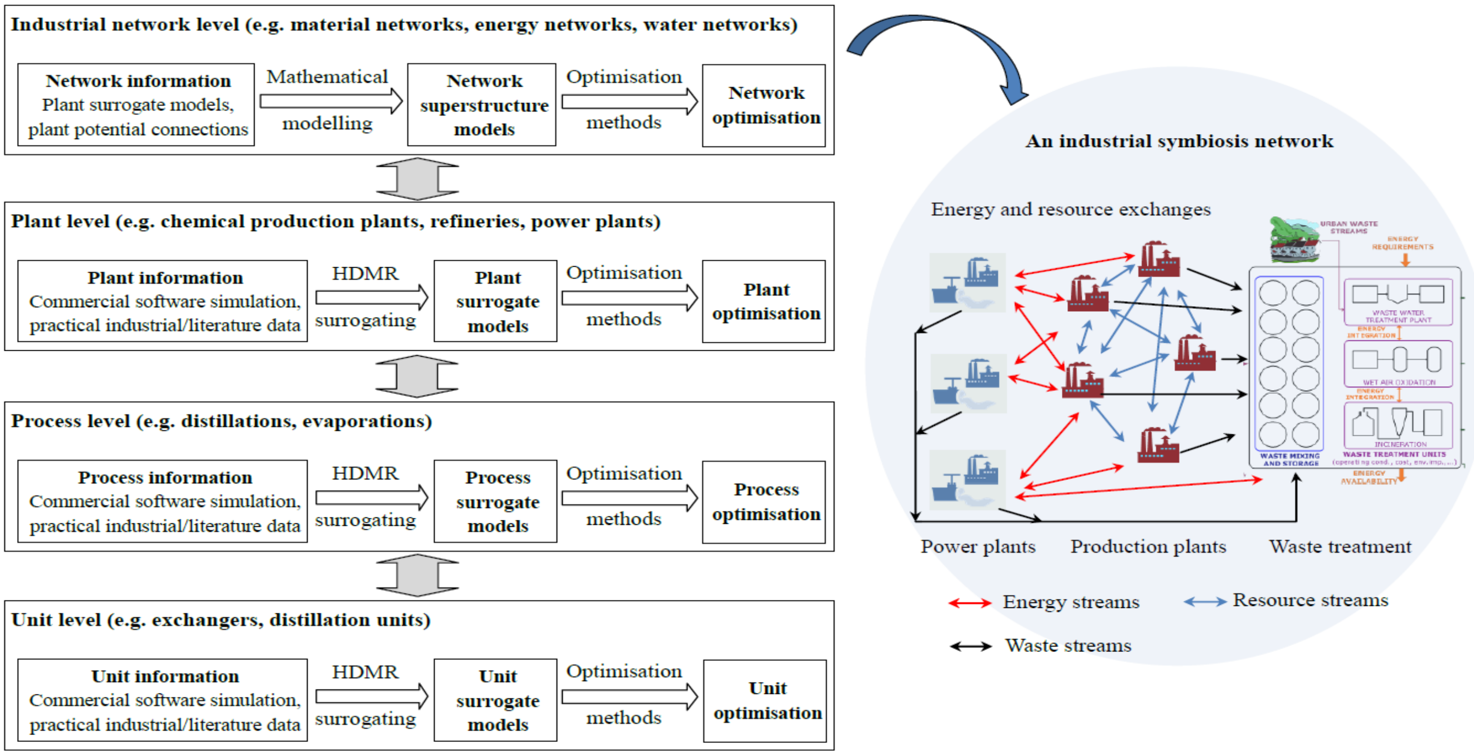
# 2.1 Hierarchy model of Eco-industrial park (Multi-level modelling)




The higher level model is composed of the models from the lower levels

1. **Advanced mathematical modelling**: the component operations at lower levels (unit level, process level and plant level) are modelled and optimised
2. **Mathematical programming:** the whole industrial symbiosis at the top level can be achieved with the optimal interaction across the resource, energy and waste networks



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# 2.2 Advanced mathematical modelling for detailed operations of units, processes and plants

In practical modelling work, detailed models of units, processes and plants are complex to be coded. All commercial simulation software packages (Aspen Plus, GateCycle, etc.) appear to the users as black boxes.

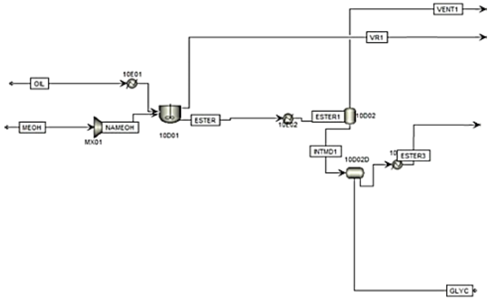
## Surrogate models:

Approximating an input-output relation using a mathematical expression, e.g. polynomials.

**Advantages**

- Enhances stability
- Reduces CPU time substantially
- while retaining accuracy.

**AspenPlus Model**



**Surrogate modelling**

**High Dimensional Model Representation (HDMR) surrogate model**

$$y \approx f(x) = f_0 + \sum_{i=1}^{N_x} f_i(x_i) + \sum_{i=1}^{N_x} \sum_{j=i+1}^{N_x} f_{ij}(x_i, x_j)$$

where $N_x$ is the number of input parameters, *i* and *j* index the input parameters, and $f_0$ is the mean value of $f(x)$



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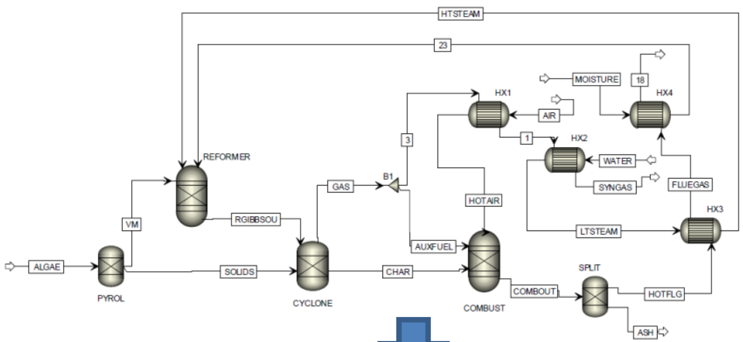
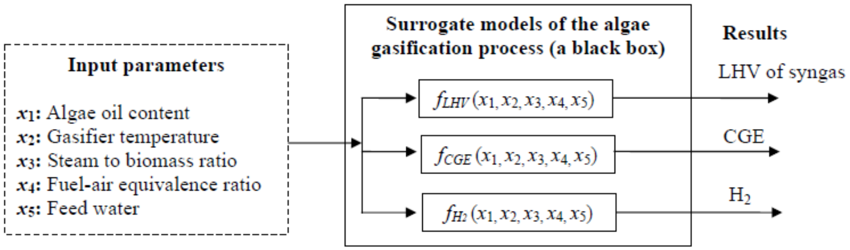
# 2.2 Advanced mathematical modelling for detailed operations of units, processes and plants

## Case 1: Chemical Process (AspenPlus)

### 1. Aspen Plus simulation




### 2. HDMR surrogate model




### 3. Surrogate formulation

$$y = C + \sum_{i=1}^{N}\sum_{k=1}^{K}\left(A_{i,k} \times x_i^k\right) + \sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=1}^{K}\sum_{n=1}^{K}\left(B_{i,j,k,n} \times x_i^k \times x_j^n\right)$$

### 4. Results

**Table 2:** *Detailed surrogate models of the algae gasification process.*

| Coefficients of Eq. (3) | LHV (MJ) | $H_2$ (kg/s) | CGE (%) |
|---|---|---|---|
| $C$ | 20.73 | 0.0532 | 1.08 |
| $A_{1,1}$ | 0.18 | 0.00057 | 0.0011 |
| $A_{2,1}$ | -0.00019 | 0.00003 | -0.00027 |
| $A_{3,1}$ | -4.84 | 0.0452 | -0.215 |
| $A_{4,1}$ | -16.02 | 0.03 | 0.167 |
| $A_{5,1}$ | -3.42 | 0.05 | -0.068 |
| $A_{1,2}$ | 0 | 0 | -0.00002 |
| $A_{2,2}$ | 0 | 0 | 1.59 |
| $A_{3,2}$ | 0 | 0 | -0.0175 |
| $A_{4,2}$ | 0 | 0 | -2.07 |
| $A_{5,2}$ | 0 | 0 | -0.071 |
| $B_{1,2,1,1}$ | 0 | 0 | 0 |
| $B_{1,3,1,1}$ | 0.0383 | 0.00042 | 0.0026 |
| $B_{1,4,1,1}$ | 0.245 | -0.00091 | -0.0114 |
| $B_{1,5,1,1}$ | 0.0242 | 0.00033 | 0.0018 |
| $B_{2,3,1,1}$ | 0.00114 | -0.00004 | 0.00005 |
| $B_{2,4,1,1}$ | 0.00486 | -0.00004 | 0.00020 |
| $B_{2,5,1,1}$ | -0.00165 | -0.00005 | -0.00007 |
| $B_{3,4,1,1}$ | 8.724 | 0.0233 | 0.375 |
| $B_{3,5,1,1}$ | -0.07 | -0.0263 | -0.00641 |
| $B_{4,5,1,1}$ | 10.95 | 0.0354 | 0.46 |
| $R^2$(coefficient of determination) | 0.98 | 0.95 | 0.90 |

**Table 3:** *Optimal solutions in three scenarios (maximisation of LHV, CGE and $H_2$ yield) based on the obtained surrogate models for the algae gasification process.*

| Solutions | Surrogate models | | | | | | Simulation results | Error (%) |
|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | Obj values | | |
| Max LHV (MJ) | 40.00 | 900 | 0.4 | 0.1 | 0.25 | 24.364 | 23.695 | 2.82 |
| Max $H_2$ (kg/s) | 40.00 | 700 | 0.8 | 0.25 | 1 | 0.1406 | 0.1363 | 3.15 |
| Max CGE (%) | 28.83 | 900 | 0.4 | 0.1 | 0.25 | 0.9206 | 0.9300 | 1.00 |



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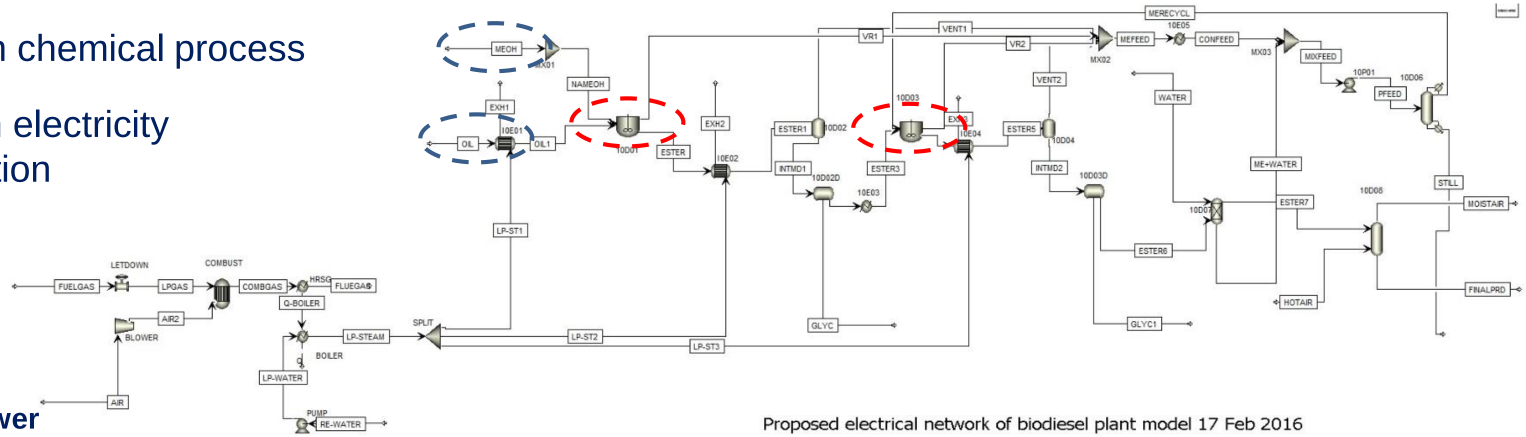
# 2.2 Advanced mathematical modelling for detailed operations of units, processes and plants

## Case 2: Chemical Process (AspenPlus) + Electrical Engineering (PowerWorld)

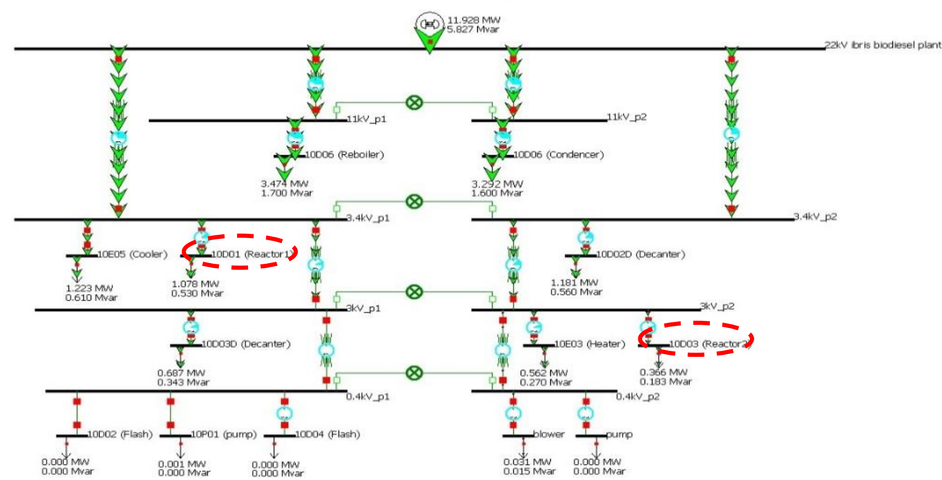
Impact on chemical process

Impact on electricity consumption



### Units that require power

| Unit | Heat duty/kW | Net work/kW | |
|---|---|---|---|
| BLOWER | | 31.1059 | blower |
| PUMP | | 0.35385 | pump |
| 10D01 | -1078.49 | | Reactor1 |
| 10D02 | 0.000261695 | | Flash |
| 10D02D | -1180.79 | | Decanter |
| 10 E03 | 562.031 | | Heater |
| 10D03 | -365.956 | | Reactor2 |
| 10D04 | -4.68E-04 | | Flash |
| 10D03D | -686.742 | | Decanter |
| 10 E05 | -1223.49 | | Cooler |
| 10P01 | 0.638225 | | pump |
| 10D06 | -3291.59 | | Condenser |
| | 3474.11 | | Reboiler |



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# 2.2 Advanced mathematical modelling for detailed operations of units, processes and plants

Case 2: Chemical Process (AspenPlus) + Electrical Engineering (PowerWorld)

## Comparison “True Model” vs Surrogate Model

| Model | Result | AP/PW model (“true model”) | cpu time/s | Surrogate model | absolute error | cpu time/s |
|---|---|---|---|---|---|---|
| Biodiesel plant(AP) | Molar flowrate (FINALPD) | 86.63 kmol/hr | 30 | 86.57 kmol/hr | -0.0007 | 16 |
| | Temperature (FINALPD) | 49.11 ℃ | | 49.12 ℃ | 0.0002 | |
| Biodiesel plant(AP+PW) | HeatDuty (10D01) | 1078.48 kW | 36 | 1075.54 kW | 0.0027 | 15 |
| | BUSPUVOLT (10D01) | 0.995 | | 0.995 | 0 | |
| | BUSANGLE (10D01) | -0.198 | | -0.197 | 0.0051 | |
| | BUSKVVOLT (10D01) | 3.383 kV | | 3.383 kV | 0 | |



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# 2.3 Mathematical programming for structuring networks at the top EIP level

Optimal interaction across the resource, energy and waste networks in industrial parks.

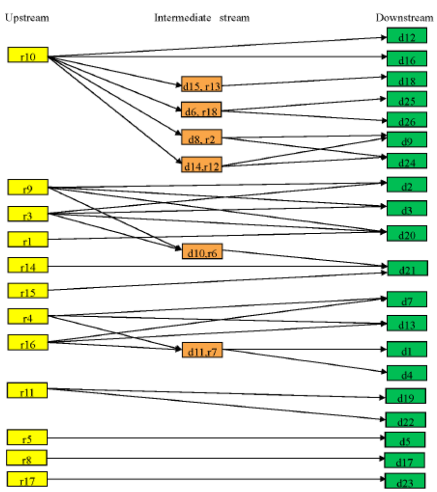
## Mathematical programming / optimisation:

An optimization problem consists of maximizing or minimizing a real function by systematically choosing input values within a set of constraints

**Advantages**

- Finding the best solution for a problem
- Efficient software tool GAMS (General Algebraic Modelling System)

**Network problems**




**Mathematical programming** →

**Mathematical programming**

$$\min/\max: z = f(x, y, \ldots)$$

$$s.t.$$

$$h(x, y, \ldots) = 0$$

$$g(x, y, \ldots) \geq 0$$

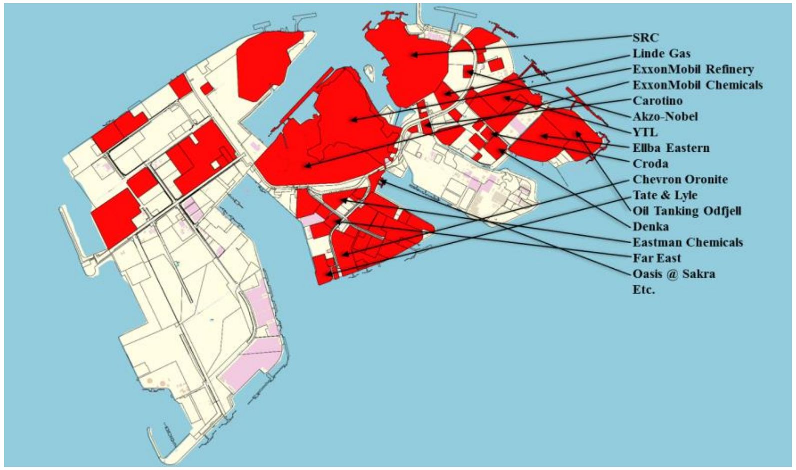
$$d(x, y, \ldots) \geq 0 \quad \ldots\ldots$$

$$x \in X, \quad y \in \{0,1\} \quad \ldots\ldots$$

where $z$ is the objective value, $f(x,y,\ldots)$ is the objective function, $x$ and $y$ are variables, $X$ is the range of $x$, and $h(\,), g(\,)$ and $d(\,)$ are constraints

# 2.3 Mathematical programming for structuring networks at the top EIP level

## Case: Material transportation network at Jurong Island




Jurong Island,

- An area of approximately 32 square kilometres.
- More than 100 companies producing a wide range of products including petroleum products, fine chemicals and pharmaceuticals
- Companies can buy and sell feedstock and products in an integration system

A new material transportation model will be built, leading to a cost efficient and environment-friendly structure

**Material network model (MILP)**

$$min\ obj = ify \times [tpc + ctax \times tce + (\sum_{\forall r \in R} \sum_{\forall d \in D} ilptc_{r,d} + \sum_{\forall rs \in R_s} \sum_{\forall ds \in D_s} iwptc_{rs,ds}) \times acf]$$

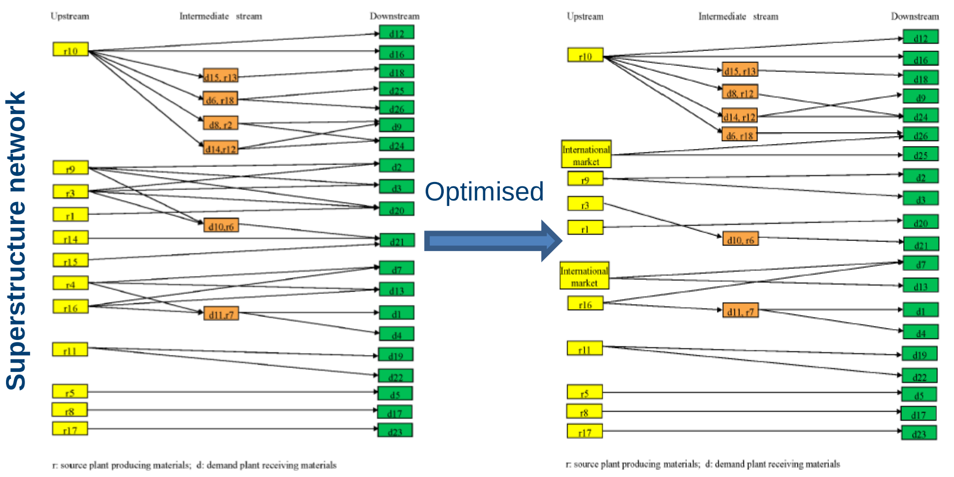
$s.t.$

$$mrt_{r,d} \le M \times rt_{r,d}, \forall r \in R, \forall d \in D,$$

$$mwt_{rs,ds} \le M \times wt_{rs,ds}, \forall rs \in R_s, \forall ds \in D_s,$$

$$mlpt_{r,d} \le M \times lpt_{r,d}, \forall r \in R, \forall d \in D, \quad \ldots\ldots..$$

**Optimisation (Min network cost and $CO_2$ emission)**



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# 2.3 Mathematical programming for structuring networks at the top EIP level

## Case: Material transportation network at Jurong Island

| | d1 | d2 | d3 | d4 | d5 | d6 | d7 | d8 | d9 | d10 | d11 | d12 | d13 | d14 | d15 | d16 | d17 | d18 | d19 | d20 | d21 | d22 | d23 | d24 | d25 | d26 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| r1 | | | | | | | | | | | | | | | | | | | | 283.8 (LP) | | | | | | |
| r2 | | | | | | | | | | | | | | | | | | | | | | | | 132.9 (S) | | |
| r3 | | | | | | | | | | 33.6 (LP) | | | | | | | | | | | | | | | | |
| r4 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| r5 | | | | | 38.8 (LP) | | | | | | | | | | | | | | | | | | | | | |
| r6 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| r7 | 35.3 (LP) | | | 10 (LP) | | | | | | | | | | | | | | | | | | | | | | |
| r8 | | | | | | | | | | | | | | | | | 202 (LP) | | | | | | | | | |
| r9 | | 68.4 (LP) | 400 (LP) | | | | | | | | | | | | | | | | | | | | | | | |
| r10 | | | | | | 87.5 (LP) | | 181 (LP) | | | | 205.8 (LP) | | 131.1 (LP) | 42.6 (LP) | 35 (LP) | | | | | | | | | | |
| r11 | | | | | | | | | | | | | | | | | | | 10.3 (LP) | | | 8.3 (LP) | | | | |
| r12 | | | | | | | | | 28.2 (LP) | | | | | | | | | | | | | | | 152.8 (S) | | |
| r13 | | | | | | | | | | | | | | | | | | 39.2 (LP) | | | | | | | | |
| r14 | | | | | | | | | | | | | | | | | | | | | 12 (LP) | | | | | |
| r15 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| r16 | | | | | | | 26.5 (LP), 386 (I) | | | | 411.5 (LP) | | 292.5 (I) | | | | | | | | | | | | | |
| r17 | | | | | | | | | | | | | | | | | | | | | | | 9.9 (S) | | | |
| r18 | | | | | | | | | | | | | | | | | | | | | | | | | 27.8 (I) | 65 (S), 509.8 (I) |

**Number (K)**: the amount of material (kt/yr) is transported with transportation K; T: truck transportation; S: short-sea transportation; LP: land pipeline transportation; I: international purchasing. E.g. **35.3 (T)**: 35.3 kt/yr of material is transported with trucks; **9.9 (S)**: 9.9 kt/yr of material is transported with ships; **400 (LP)**: 400 kt/yr of material is transported with land pipelines; **27.8 (I)**: 27.8 kt/yr of material is purchased from international market.

**Transportation tools:**

Trucks: 

Ships: 

Pipelines: 

**Table 9:** *Comparison of the optimal solutions under different life times.*

| Project life times (years) | Transport cost per year ($10^3 \times \$/yr$) | Material purchase cost per year ($10^9 \times \$/yr$) | Pipeline installing cost ($10^6 \times \$$) | $CO_2$ emission per year (t/yr) | Total cost related to transportations ($10^6 \times \$$) 1 year | 10 years | 50 years | 100 years |
|---|---|---|---|---|---|---|---|---|
| 1 | 766.04 | 5.02 | 0 | 1072.4 | 0.77 | 7.66 | 38.3 | 76.6 |
| 10 | 130.74 | 5.02 | 1.47 | 245.1 | 1.60 | 2.77 | 8.00 | 14.54 |
| 50 | 38.80 | 5.02 | 3.39 | 125.4 | 3.43 | 3.78 | 5.33 | 7.27 |
| 100 | 34.87 | 5.02 | 3.62 | 120.3 | 3.66 | 3.97 | 5.37 | 7.11 |



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# 2.4 Modelling and optimisation methods for eco-industrial parks

## Summary:

1. At unit level, process level and plant level, the operations of units, processes and plants can be modelled and optimised using advanced mathematical modelling methods (surrogate models)
   - **Chemical processes (min waste)**
   - **Chemical processes + Electrical engineering (min power consumption)**
   - **Chemical processes including detailed unit operations (future)**
2. At the top level (industrial networks), the whole industrial symbiosis can be achieved with the optimal interaction across the resource, energy and waste networks using mathematical programming methods
   - **Material transportation network (min cost and $CO_2$ emission)**
   - **Resource exchanging network (future)**
   - **Energy network (future)**
   - **Water network (future)**

**Next step: applying the proposed mathematical modelling and optimisation methods to the integrated industrial park system**



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# 3. System integration for eco-industrial parks





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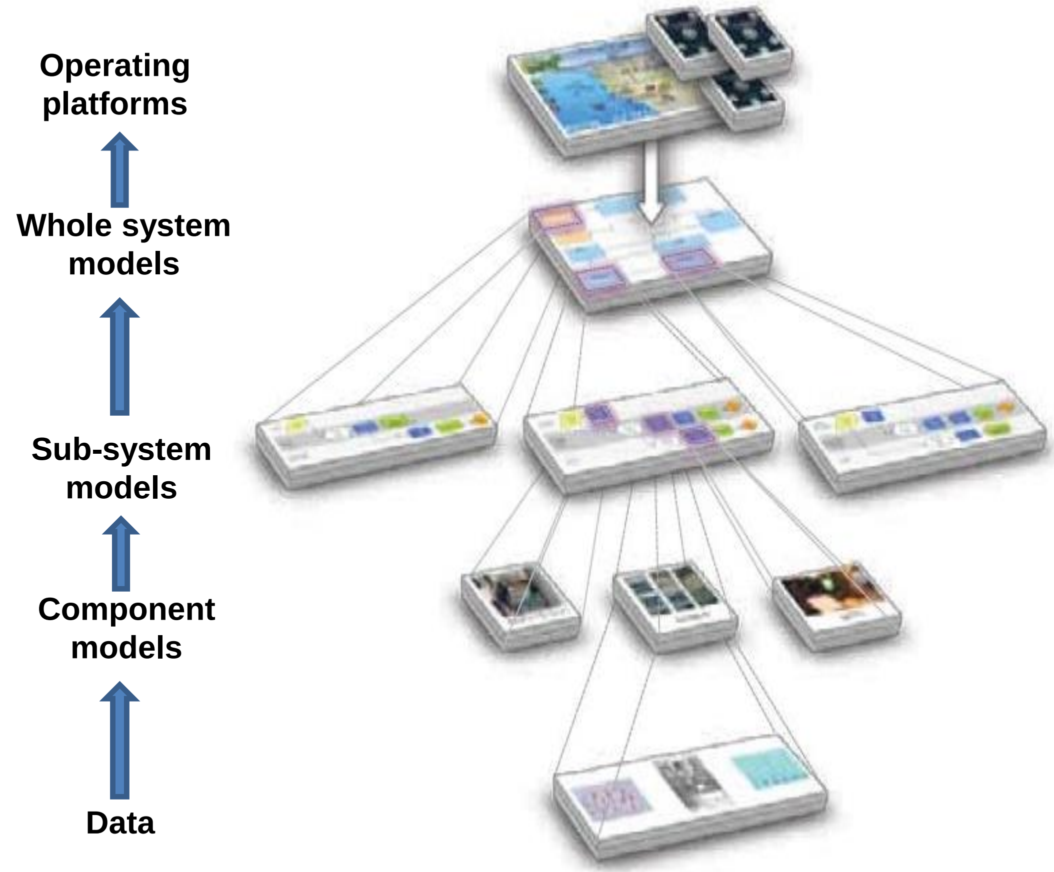
# 3.1 System architecture for eco-industrial parks

The application make use of the latest advances in **semantic technologies**

- Represent components by surrogate models
- Associate each industrial component with its data and own semantic representation
- Combine component models into sub-system models which are described as sub-system ontologies
- Build the overall ontology to link all sub-system ontologies
- Use query engine to read the industrial park information from the overall ontology, and solve industrial problems



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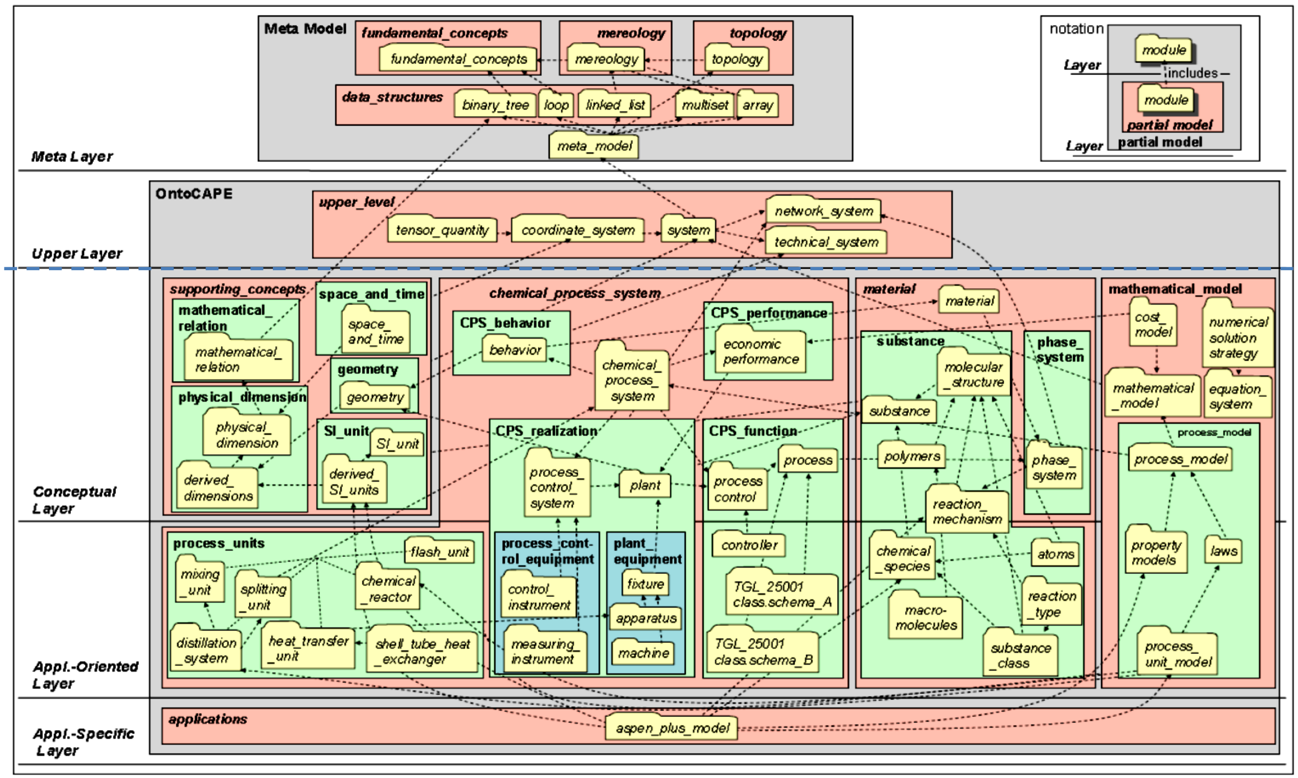
# 3.2 System representation for eco-industrial parks (ontologies)

**OntoCAPE is a large-scale ontology for the domain of Computer-Aided Process Engineering (CAPE)**

- It shares common understanding of the structure of information among people or software agents
- It includes 62 sub-ontologies which can be used individually or as an integrated suite.
- The sub-ontologies are organized across different abstraction layers, which separate general knowledge from knowledge about particular domains and applications.

**Extendable**
(can be extended to other domains)

**Specific application**
(chemical processes)



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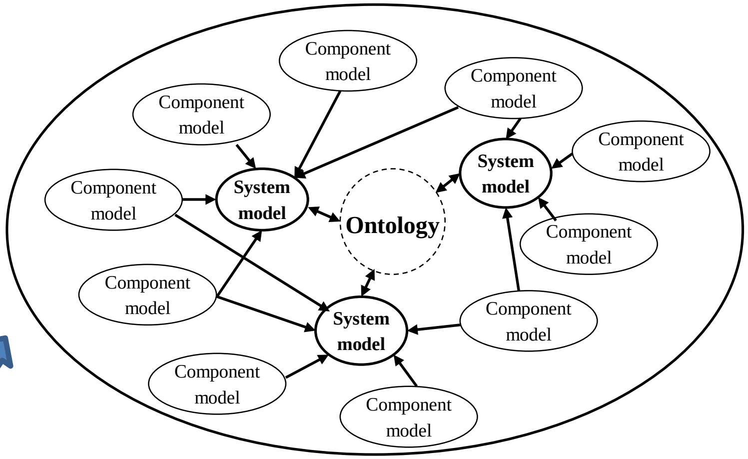
# 3.2 Eco-industrial park (system integration)

**Jurong Island**

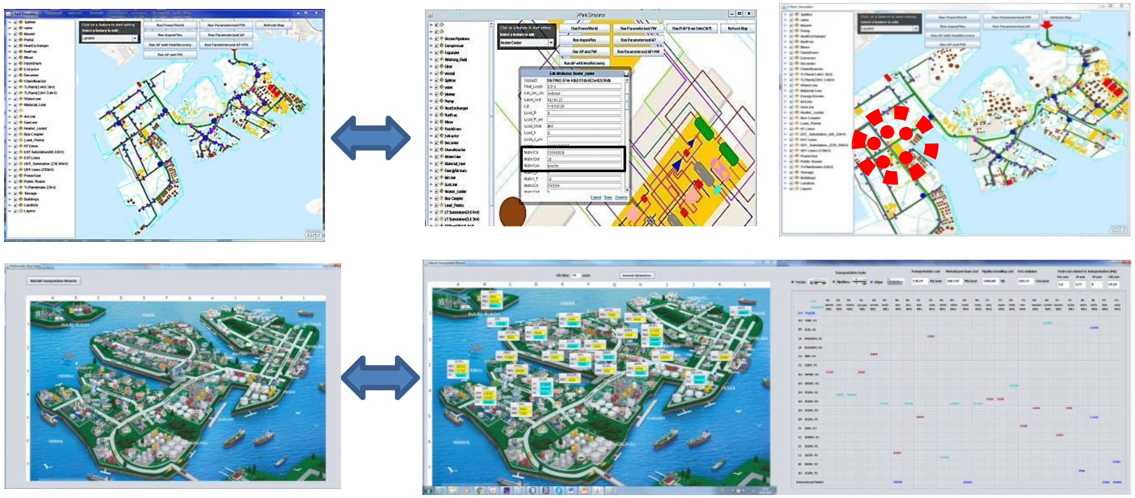
**Data**

**Knowledge Base (Semantics)**

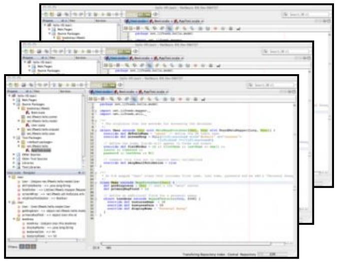



**Data, Models**

**Operating platforms**



**Querying Engines (Java programming)**



**Results**

**Solvers**

GAMS

aspentech

MathWorks

MoDS

**Solvers**

……



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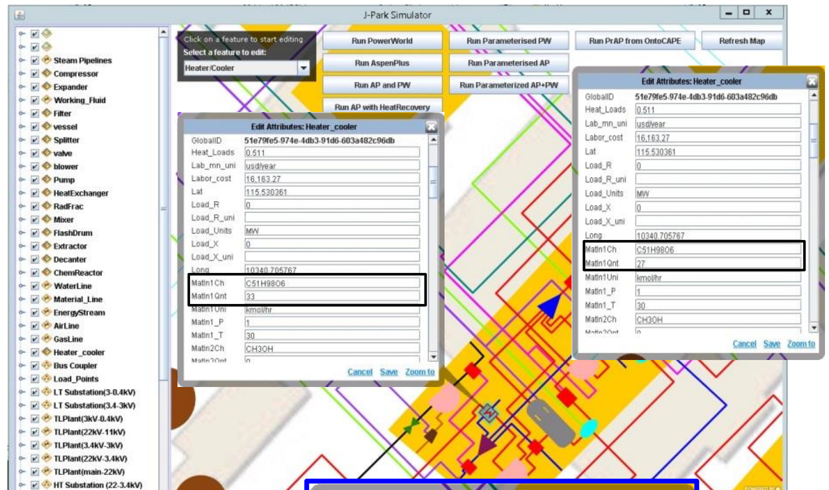
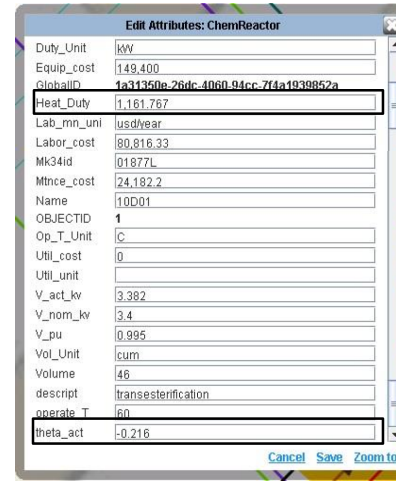
# 3.3 Eco-industrial park (operating platform on ArcGIS)

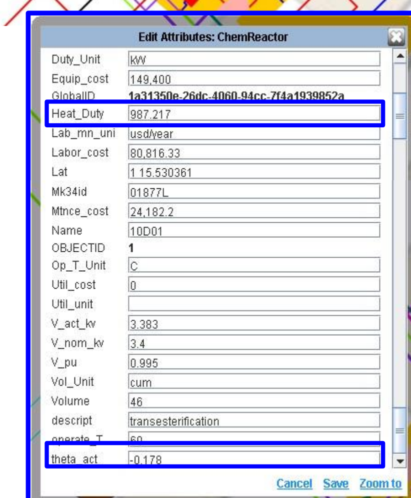
## Simulation of Chemical Process and Electrical Engineering (Case 2)

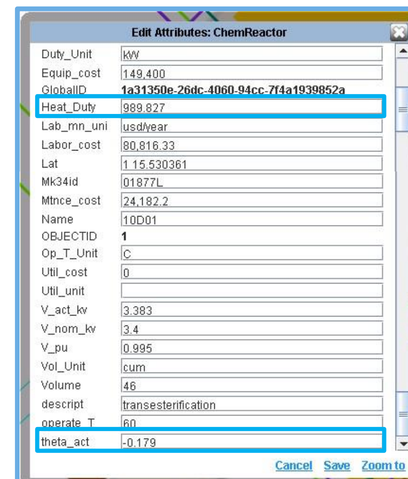
**JParkSimulator (ArcGIS)**




Chemical Process Simulation with the consideration of power network



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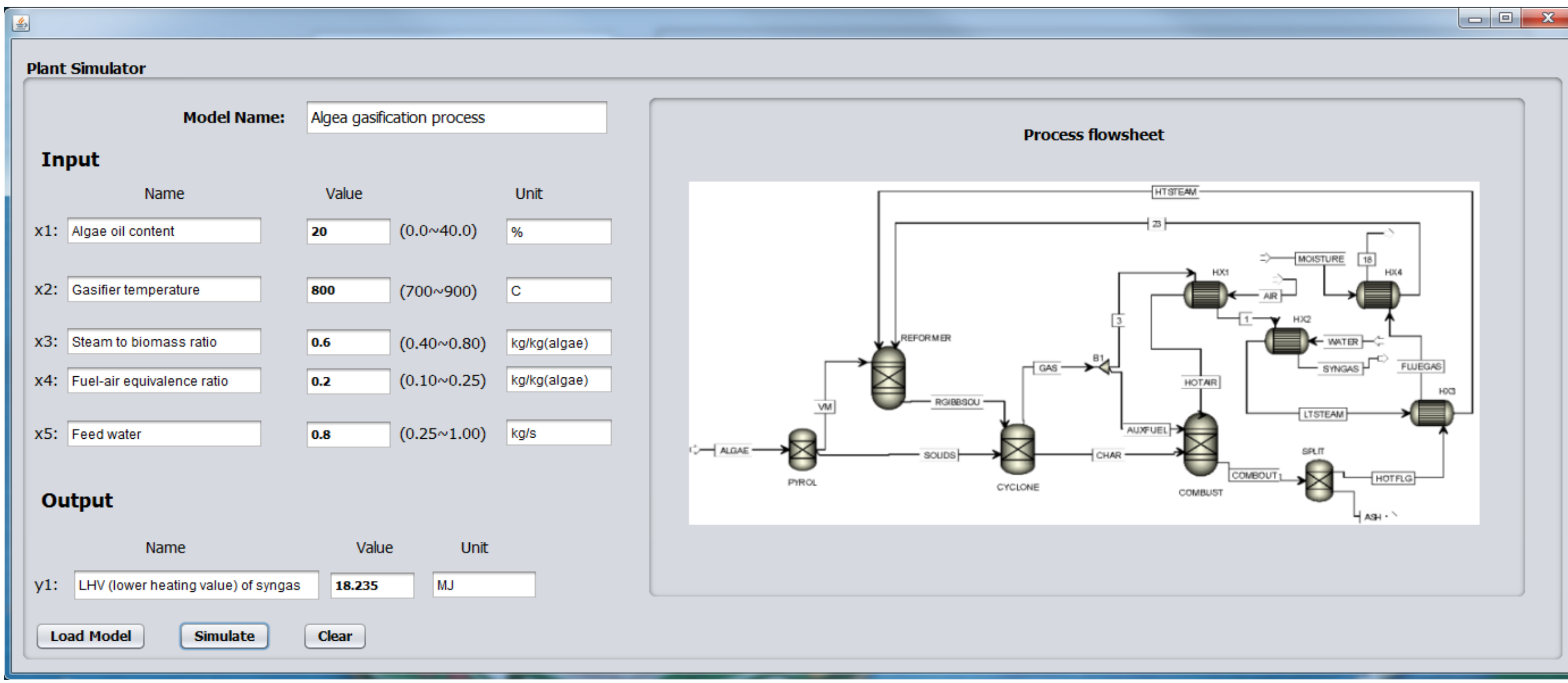
# 3.4 Eco-industrial park (other operating platforms)

## Chemical Process Simulation (Case 1)

**Jpark**



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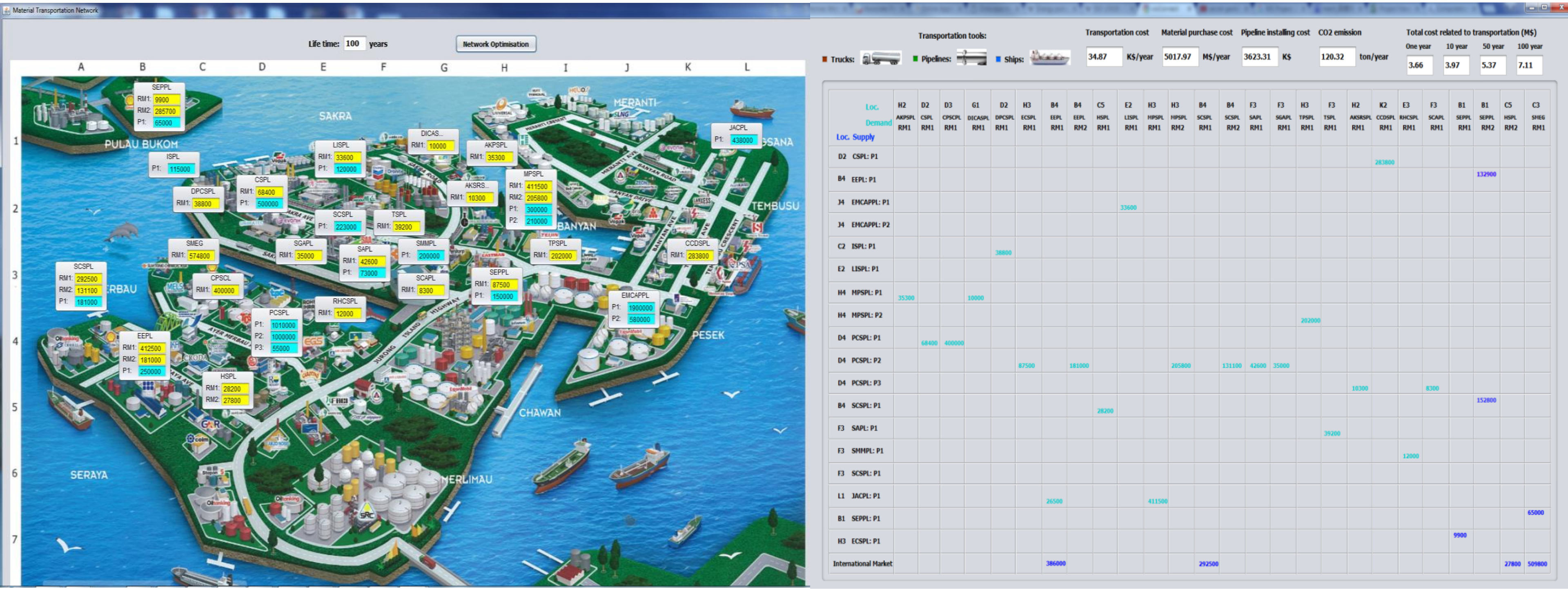
# 3.5 Eco-industrial park (other operating platforms)

## Material transportation network optimisation (Case 3)

**Jpark**

**A smart network can achieve dynamic optimisation**



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# 3.6 System integration for eco-industrial parks

## Summary:

Integrated system platforms have been developed for eco-industrial parks

- **Store industrial parks' information**
- **Simulate chemical processes**
- **Simulate chemical processes with power supply**
- **Optimise material transportation network in industrial parks**
- **Energy network in industrial parks (future)**
- **Water network in industrial parks (future)**
- **Resource and energy network in industrial parks (future)**



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# 4. Conclusions and future works



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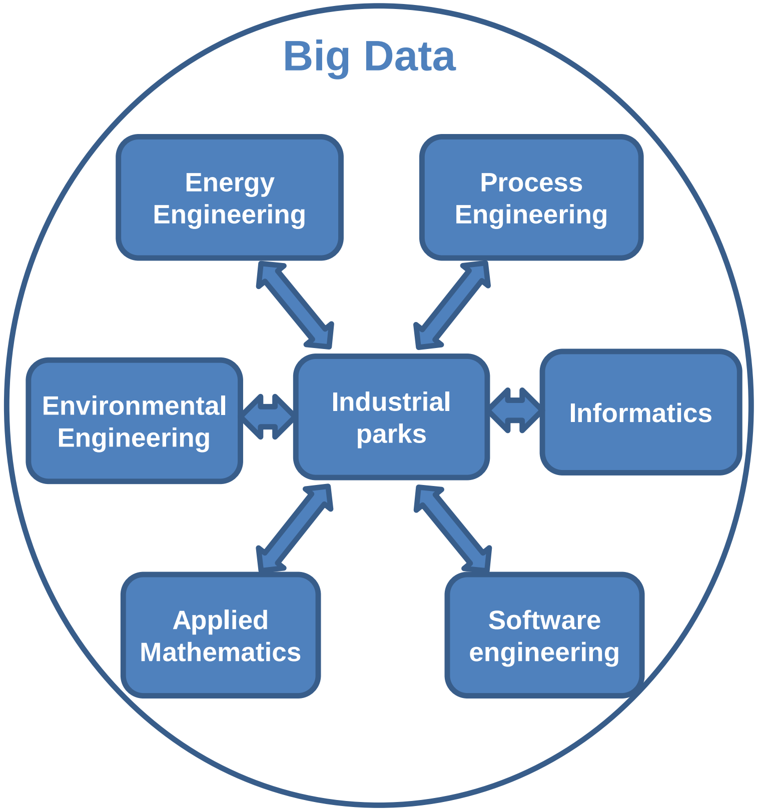
# 4.1 Conclusions




**Modelling and optimisation for eco-industrial parks**

- Hierarchy model (four levels)
- Surrogate models for lower level operations and optimisation
- Mathematical programming for top level optimisation
- Ontologies for representing the knowledge base of industrial parks
- Java Query for system and software integration
- Operating platform for smart industrial park



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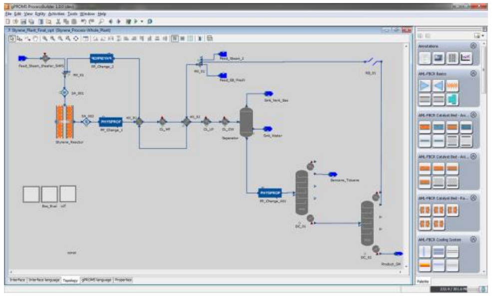
# 4.2 Future work

## Parametrisations for more plants and processes

### gPROMS platform:

- create high-fidelity custom models of processes
- apply these within a powerful optimisation framework to seek optimal design and operating solutions directly
- solve the resulting large-scale mathematical problem rapidly and robustly

**gPROMS Model**



**Surrogate modelling**

**High Dimensional Model Representation (HDMR) surrogate model**

$$y \approx f(x) = f_0 + \sum_{i=1}^{N_x} f_i(x_i) + \sum_{i=1}^{N_x} \sum_{j=i+1}^{N_x} f_{ij}(x_i, x_j)$$

where $N_x$ is the number of input parameters, *i* and *j* index the input parameters, and $f_0$ is the mean value of $f(x)$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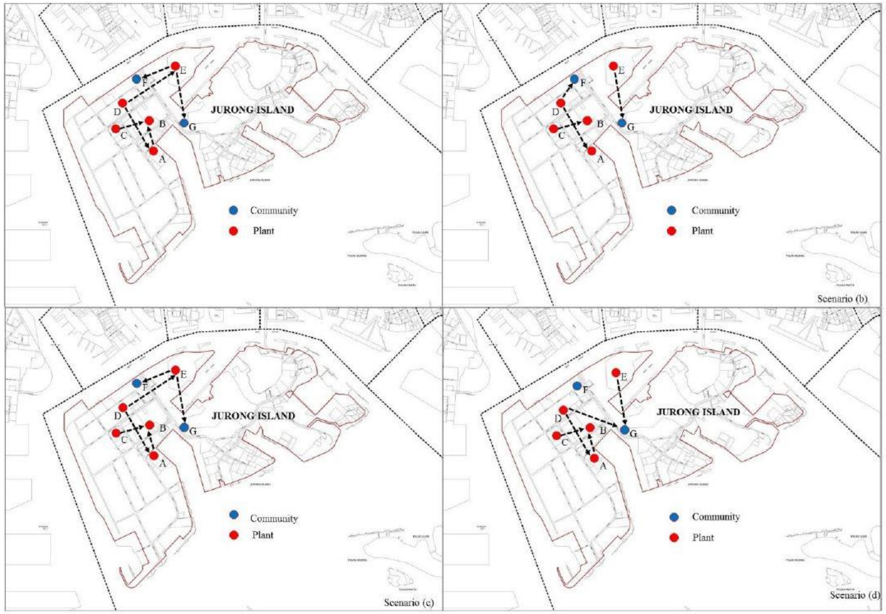
# 4.2 Future work

## Inter-plant Waste Heat Optimisation


- ZEON Chemical — butadiene rubber
- Lanxess — butyl rubber
- Air Liquide — air separation
- ExxonMobil — hydro cracking
- Ibris Bio-Fuels — biodiesel



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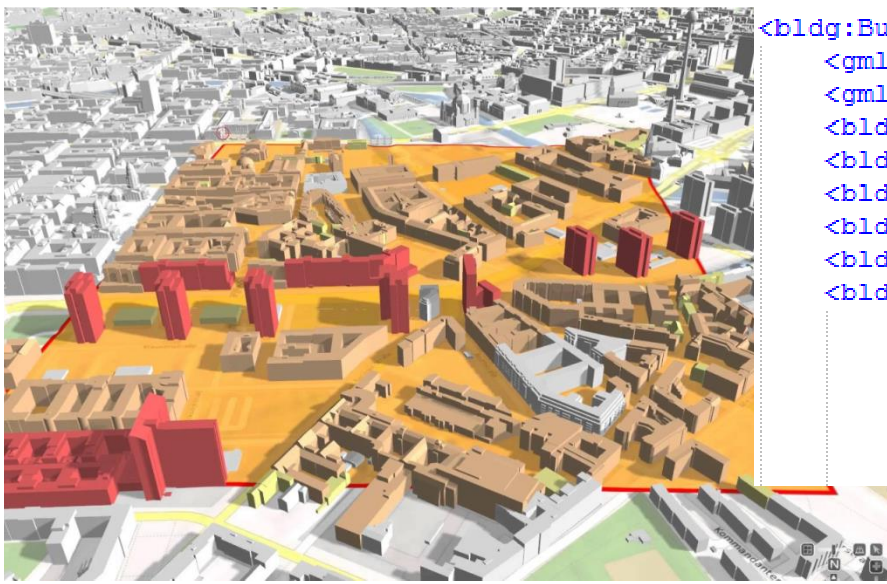
# 4.2 Future work

## CityGML

- Enables representation of 3D objects.
- Enables interaction with 3D objects.
- Adds semantic properties to 3D objects.



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    <gml:description/>
    <gml:name> b_12529I1</gml:name>
    <bldg:class/>
    <bldg:function>2729</bldg:function>
    <bldg:usage/>
    <bldg:roofType/>
    <bldg:measuredHeight uom="#m">8.0</bldg:measuredHeight>
    <bldg:lod1Solid>
        <gml:Solid>
            <gml:exterior>
                <gml:CompositeSurface>
                    <gml:surfaceMember>
                        <gml:OrientableSurface orientation="+">
```



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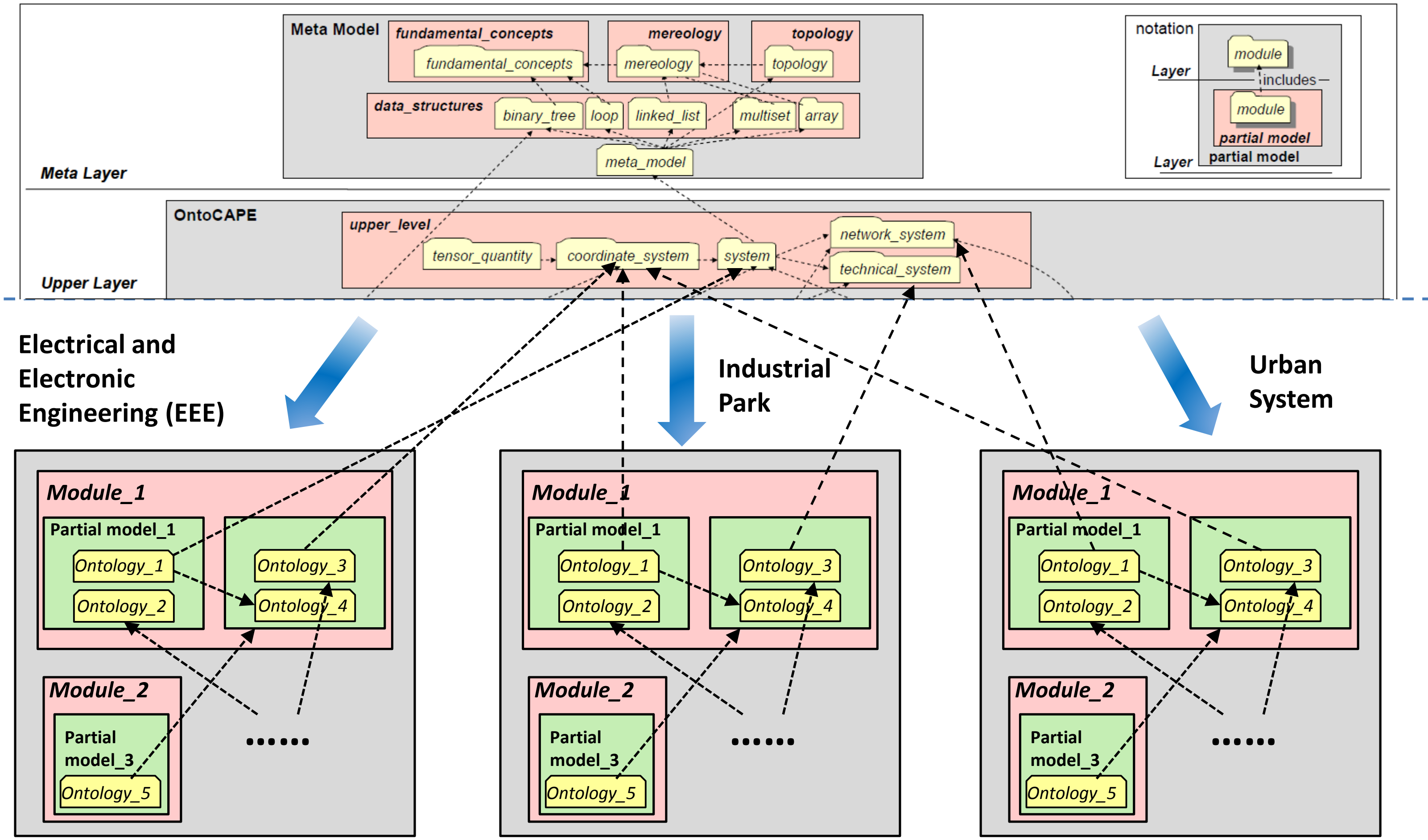
# 4.2 Future work

## Ontology based framework (OntoCAPE extension)

**Extendable**
(OntoCAPE can be extended to other domains)

**Specific domain applications**





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# CAM.CARES - IRP 3: Carbon Abatement in the Petroleum Refining Industry: A Control and Optimisation Research Network (CAPRICORN)

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