

Logistic Optimization for Renewable Energy Carriers

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Abstract: We describe a tool for the simulation and optimization of a EU-wide multi-echelon logistics network. In particular we evaluate the feasibility and profitability of a de-centralized approach to biofuel production from residual biomass on an EU-wide level. The overall objective of the FP7 project BioBoost¹ was “[...] to pave the way for de-central conversion of residual biomass to optimised, high energy density carriers, which can be utilised in large scale applications for the synthesis of transportation fuel and chemicals or directly in small-scale combined heat and power (CHP) plants”. One of the sub-goals was the development of a software tool for the simulation of different scenarios of utilization and for the optimization of logistics. The resulting software has been used to calculate optimized scenarios that can be explored online via the BioBoost Navigator² and is now available as open-source software for application to similar optimization problems.

Keywords: 2nd generation biofuels, logistics optimization, simulation-based optimization

1 Modeling

An essential part of solving large problems such as international multi-modal multi-echelon logistic networks is carefully choosing a suitable level of abstraction and corresponding sources of information. In the case of BioBoost, the task was to collect residues or waste materials economically by using several aggregation and transformation steps. In a general, very simple formulation the problem could be modeled as a set of locations where source material i.e. feedstock can be obtained, is then transported to intermediate processing plants and further transported to its final destination where it is upgraded to a consumer product. This is shown in Figure 1, where first, feedstock is collected e.g. straw from the fields to a local depot, where it is further transported to de-central conversion facilities, where the energy density is increased, mostly by reducing oxygen content. Then, the resulting energy carrier is transported to the central facilities where it is converted to its final form, e.g. transport fuel or heat and power.

¹ <http://bioboost.eu> This work is based on results of the BioBoost project and contributions from all consortium members. BioBoost ran from 1-2012 to 6-2015 and was funded under contract 282873 within the Seventh Framework Programme by the European Commission.

² <http://iung.neogis.pl/navigator/>

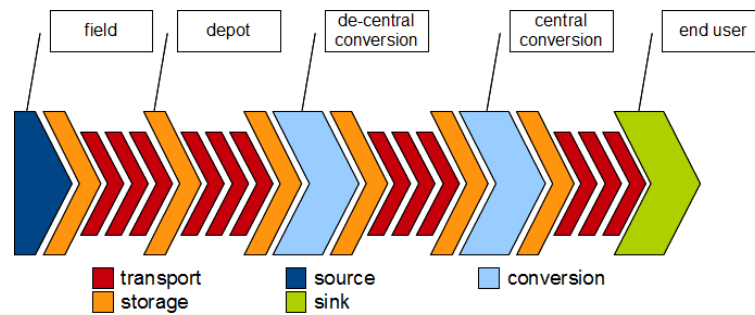


Figure 1 Logistic Chain

Beside this simple logistic chain, several additional effects have to be considered. First, obtaining different amounts of feedstock probably has a non-linear effect on the price, i.e. buying all available source material from on source location will probably drive prices up. On the other side, a high demand favours cost-efficient equipment and procurement processes which might reduce handling and transport costs. Moreover, when logistic networks that span multiple countries are considered, different cost factors such as labor, fuel or investment costs might differ significantly between locations. Most importantly, the level of aggregation and hence the sizes of intermediate and final processing facilities have a large effect on the economy of scale, i.e. larger facilities are much more cost effective. On the other hand, larger facilities probably require longer and, hence, more expensive delivery of source material.

In the BioBoost Project the following factors have been considered:

- | | |
|--|--|
| • feedstock/source locations | – investment |
| • intermediate conversion locations | – fuel |
| • final conversion locations | – labor |
| • transport distances between all locations | • economies of scale for different conversion technologies and different plant sizes |
| • transport means and modes (chosen per single transport) | • estimated regional feedstock price based on |
| – costs for transport and handling per ton and per kilometer | – current market volume and regionally established price |
| • storage costs for different feedstock and storage types | – potential market volume |
| • feedstock potentials for all source locations | – expected price increase according to expected demand |
| • cost scaling factors per region for | |

In summary many different factors have to be considered, each with many different possibilities and these must be counterbalanced against each other to arrive at a viable and cost effective solution.

1.1 Model Simplifications

In order to estimate the viability of many different scenarios, the calculation had to be simplified without sacrificing accuracy. This was achieved with the elimination of several parameters and reduction of number of parameter choices so that effectively fewer scenarios are possible. This was done in a way, that only inferior scenarios were ruled out. Moreover, the calculation of these scenarios has been aggregated to a reasonable granularity to allow very fast calculation on a computer.

1.1.1 Regional Aggregation

To limit the number of locations in a meaningful way, the smallest territorial unit that is standardized throughout the European Union was used as a reference. The EU-Nomenclature of Units for Territorial Statistics [NUTS] has several granularity levels of which NUTS-3 is the finest, examples are the Austrian *Bezirke*, German *Landkreis*, French *Département*, Italian *Province*. The large difference in the size of the NUTS 3 regions led to a distorted distance matrix as intra-regional transport was in some cases several times longer than inter-regional transport, which impacted the optimisation. Accordingly, the geographical size was limited to a maximum of 7500 km² by dividing large regions, giving about 2000 regions in the European Union.

1.1.2 Temporal Aggregation

To further reduce computational complexity all estimates are based on yearly averages. Beginning from the estimated yields of feedstock in every region, over transport and storage cost for yearly amounts up to construction and operation costs of conversion facilities based on yearly depreciation and yearly average costs.

1.1.3 Implicit Parameter Selection

Finally, several parameters can be implicitly selected, based on the choices already made for other parameters. Most importantly, the sizes of all facilities have been eliminated from the list of free variables by automatically determining appropriate sizes. This was made possible by the incremental evaluation of each scenario. Effectively, only the amount of feedstock as ratio of available feedstock per region has to be selected, together with the target region for each source region for every type of transport, i.e. once for feedstock and once for intermediate product. The accumulated amounts in a region thereby determine the size of the facility. For example, if region A yields 10kt/a and region B yields 20 kt/a and all feedstock is bought and transported to region C, a total of $10+20 = 30$ kt/a will be in region C for further processing. Taking into account a certain downtime for maintenance a plant with a yearly turnover of a little bit more than 30 kt/a is built.

1.2 Formalization

The following formulates and succinctly summarizes all calculations performed in the implementation of the model.

Quantities at source

$$Q_{p,r}^s = P_{p,r}^f \cdot \mathbf{u}(\mathbf{p}, \mathbf{r})$$

Feedstock Acquisition Cost

$$C_{p,r}^f = P(p, r) \cdot Q_{p,r}^s$$

Transport Cost

$$C_{p,r}^t = Q_{p,r}^s \cdot D_{r,t(p,r)} \cdot \frac{P_{p,r}^t + P_{p,t(p,r)}^t}{2}$$

Handling Cost

$$C_{p,r}^h = Q_{p,r}^s \cdot (P_{p,r}^h + P_{p,t(p,r)}^h)$$

Quantities at Target

$$Q_{p,r}^t = \sum_{\text{src} \in \text{NUTS}} Q_{p,\text{src}}^s \cdot \delta_{t(p,\text{src}),r}$$

Optimized Plant Capacities

$$CP_{p,r}^c = \frac{Q_{p,r}^t}{P_p^{\text{uf}}}$$

Variable Conversion Cost

$$C_{p,r}^v = Q_{p,r}^t \cdot P_{p,r}^{\text{cv}}$$

Scaled Plant Maintenance Cost

$$C_{p,r}^m = \left(\frac{CP_{p,r}^c}{P_p^{\text{ds}}} \right)^{\sigma^{\text{mc}}} \cdot P_{p,r}^{\text{mc}}$$

Scaled Plant Construction Cost

$$C_{p,r}^c = \left(\frac{CP_{p,r}^c}{P_p^{\text{ds}}} \right)^{\sigma^{\text{cc}}} \cdot P_{p,r}^{\text{cc}}$$

Financing Cost $C_{p,r}^i = \lambda \cdot C_{p,r}^c$

Storage Capacity $CP_{p,r}^s = CP_{p,r}^c \cdot \frac{P_p^{\text{ss}}}{365}$

Storage Cost $C_{p,r}^s = CP_{p,r}^s \cdot P_p^{\text{sc}}$

Produced Quantities at Source (for next logistics echelon)

$$Q_{p',r}^s = Q_{p,r}^t \cdot \gamma_{p,p'}^{\text{cy}}$$

Revenue $R_{p,r} = Q_{p,r}^s \cdot S_p^s + Q_{p,r}^t \cdot S_p^t$

Total Cost

$$C = \sum_{p \in \text{Products}} \sum_{r \in \text{NUTS}} C_{p,r}^f + C_{p,r}^t + C_{p,r}^h + C_{p,r}^v + C_{p,r}^m + C_{p,r}^c + C_{p,r}^i + C_{p,r}^s - R_{p,r}$$

Purchase Price

$$P(p, r) = P_p^b \cdot \left(\frac{\exp(\sigma_p^p) - P_p^{\text{max}}}{\exp(\sigma_p^p) - 1} + \frac{\exp(\sigma_p^p \cdot \mathbf{u}(\mathbf{p}, \mathbf{r})) \cdot (P_p^{\text{max}} - 1)}{\exp(\sigma_p^p) - 1} \right)$$

	Index Variables	Unit
p	product	[product]
r	region	[region]
	Facts	
NUTS	set of regions	[{region}]
Products	set of products	[{product}]
S_p^s, S_p^t	product p 's sales price (at source s or at target t)	[€]
$D_{\text{src,dst}}$	distance matrix (route lengths)	[km]

$P_{p,r}^f$	feedstock potentials for product p and region r	[t/a]
$P_{p,r}^{\text{cv}}$	regional product conversion cost (per ton of feedstock)	[€/t]
$P_{p,r}^{\text{mc}}$	regional plant maintenance cost (for the whole plant per year)	[€/a]
$P_{p,r}^{\text{cc}}$	regional plant construction cost (for the whole plant per year)	[€/a]
$P_{p,r}^{\text{sc}}$	regional product/plant storage cost	[€/t/a]
P_p^{ds}	plant design size	[t/a]
P_p^{uf}	plant design utilization factor	[1]

p_p^{ss}	product/plant safety stock duration	[days/a]
$p_{p,r}^t$	regional product transport costs	[€/t/km]
$p_{p,r}^h$	regional product handling costs	[€/t]
$\gamma_{p,p'}^{cy}$	conversion yield factor / mass rate for conversion of product p into p'	[t/t]
σ^{cc}	size-dependent construction cost scaling factor	[1]
σ^{mc}	size-dependent maintenance cost scaling factor	[1]
λ	interest rate	[%/a]
Variables (optimization targets)		
$u(p,r)$	feedstock utilizations	[1/a]
$t(p,r)$	product transport targets	[region]
Intermediate Results		
$Q_{p,r}^s$	quantities or amounts at source and at target, respectively	[t/a]
$Q_{p,r}^t$		
$CP_{p,r}^c$	converter capacities	[t/a]
$CP_{p,r}^s$	storage capacities	[t/a]

$C_{p,r}^c$	construction cost	[€/a]
$C_{p,r}^f$	feedstock purchase cost	[€/a]
$C_{p,r}^i$	investment cost	[€/a]
$C_{p,r}^m$	maintenance cost	[€/a]
$C_{p,r}^s$	storage cost	[€/a]
$C_{p,r}^t$	transportation cost	[€/a]
$C_{p,r}^h$	handling cost	[€/a]
$C_{p,r}^v$	variable conversion cost	[€/a]
$P(p,r)$	purchase price	[€]
p_p^b	base price per ton of product	[€/t]
p_p^{\max}	maximum price multiplier (for 100% market saturation)	[1]
σ_p^p	price curve scaling factor	[1]
$R_{p,r}$	revenue	[€/a]
Result		
C	total cost	[€/a]

1.3 Support data

Three conversion pathways are included in the optimisation model. The Karlsruhe Institute of Technology developed the Bioliq- or **Fast Pyrolysis (FP)-process**. Straw is pyrolysed at 500°C in the absence of oxygen to char and vapours, which are rapidly cooled down and are mixed with the milled char to a slurry. It contains 85 % of the straw energy but has only 12% of its volume, enabling railway transport. Off-gases are burned to provide the pyrolysis heat. The drop-in transportation fuels are produced in a large, central plant with a feedstock demand between 1.3 and 4 million tonnes of biosyncrude, which relates to a thermal fuel capacity between 800 MW to 2.5 GW. The slurry of 5 to 15 FP-plants is gasified at high pressure and temperatures of over 1200 °C to hydrogen and carbon monoxide for fuel production via Methanol-to-Gasoline- or Fischer-Tropsch-synthesis with green power as co-product. These are expected to have a GHG-avoidance potential of 81 % compared to fossil fuels.

The **Catalytic Pyrolysis- (CP) pathway** is based on the CatOil-technology developed by CERTH (Center for Research and Technology Hellas), Royal DSM and Neste. Forest residues are dried and grinded and pyrolysed at about 500 °C in absence of oxygen in contact to a catalytic material. Compared to FP the catalyst splits off a higher share of the oxygen which is contained in the biomass molecules (about 45 % by weight) as carbon dioxide, carbon monoxide or water. The pyrolysis vapours are rapidly cooled. The condensed biooil contains 50 % of the liquid biomass energy, is low in oxygen content (15 to 20 %) and has a heating value of about 30 GJ/t. CFP off-gases and the catalyst coke are combusted to supply the reaction heat for pyrolysis and produce power. A truck load (25 t) of forest fuel

yields 4.5 tonnes biooil, which can be railway-transported to a refinery. The upgrading includes alternating steps of separation and hydrotreatment, yielding by-products acetic acid, phenol and light gases. Separation of the first two reduce the hydrogen consumption, the light gases could either be marketed as green LPG or recycled to hydrogen generation. Due to changes in the European refining sector it is expected that the CP biooil may replace 2 % of fossil crude. This enables use of existing capacity for steam methane reforming and hydrotreatment for the deoxygenation of the biooil. The product is co-processed with the fossil streams and distilled to the conventional transportation fuels gasoline/kerosene/diesel according to the production slate of the refinery. All fuels purely consist of hydrocarbons which guarantee drop-in blending. The fuels are fully engine compatible and do not require changes in the distribution infrastructure, two points very important for consumer acceptance. The fuels have a GHG-avoidance potential of 81 % compared to fossil fuels.

The **Hydrothermal Carbonisation (HTC) process** was developed by AVA-CO₂. Organic municipal waste with a typical composition of 60 to 70% water and about 15% ash is minced and heated with steam to about 180 to 250 °C at 10 bar. The biomass is converted to HTC biocoal by elimination of chemically bonded water from carbohydrates (dehydration). After several hours the pressure is released in an expansion vessel leading to a separation of wet biocoal and steam. The steam is used to start the exothermal reaction in the next reactor. During HTC all soluble salts are solved and found to a high share in aqueous solution after the reaction. This lowers the potassium content of HTC coal which increases the ash melting temperatures from about 700 °C to 1200 °C for organic waste based biocoal. Low K⁺ and Cl⁻ content allow combustion of non-wood biomass in power plants because slagging and corrosion problems are avoided. The wet biocoal can be filter-pressed to a water content of 50 to 60 %. The HTC process has an energetic conversion efficiency of 75 % from organic waste to biocoal.

Biomass potential and feedstock price

The utilization of organic waste from kitchen, garden or food production is considered environmentally sustainable *per se*. These are currently combusted at high costs (due to 60 to 80% water content) or composted. The forest residue potential included only those amounts from final fellings (branches, tree-tops, bent and rotten stem wood), stand maintenance (thinning wood), stumps (where permitted) and wood from roadsides or land management, which could be extracted without compromising soil fertility or environmental protection aims. Forest residues are typically left in the forest to rot or a certain share is used as fuel for heating or power generation in some countries. Concerning straw, the soil demand for organic matter and straw applications in agriculture (for fodder, bedding, tulip covering) were deducted from the theoretical potential. This surplus straw is typically ploughed under, its rotting consumes nitrogen fertiliser and is in some cases adverse to soil fertility. In some countries a certain share is used for heat and power generation. So if the optimisation model sources 100% of the feedstock it is still the sustainable part of ready available residue

biomass. No feedstock is diverted from the production of food, feed, timber, pulp or wood boards.

Feedstock costs were determined assuming use of most efficient equipment and procurement processes, which are not necessarily operated in all regions today but are required to fuel facilities with a feedstock demand in the range of tens to hundreds of thousand tonnes biomass. The price depends on offer and demand in a free market. For sourcing between 0 and 50 % of the sustainable and available feedstock a single price is assumed, which increases with higher utilization rates as shown in the figure below for the European average. Feedstock-competing sectors (wood pellets, straw building) are expected to profit initially from an increased demand due to establishment of more efficient procurement technology until prices generally increase at higher sourcing ratios as observed on the Swedish forest fuel market.

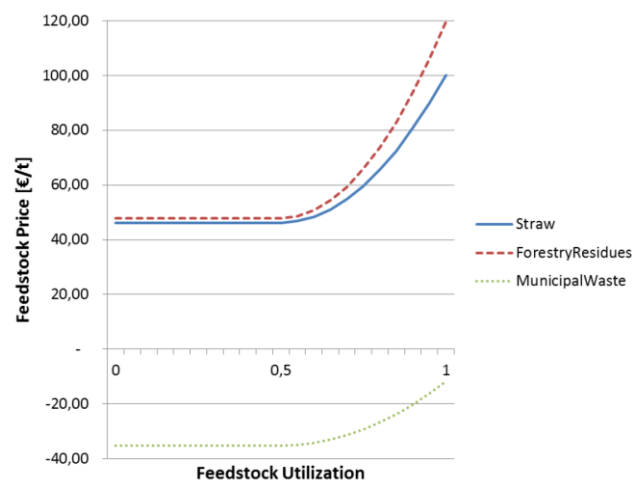


Figure 2: The feedstock prices (y-axis) depend on degree of utilization (x-axis). Increasing prices were assumed, if more than 50% of the available residue and waste feedstock is marketed.

Transport distance matrix

For the determination of transport costs, the distances between feedstock source (e.g. field-side pile) and de-central conversion plant is required. Average route lengths were determined on base of the European road network using Open Street Map data. If feedstock and conversion plant are in the same region, an average route length was estimated by calculating routes from 20 random points in the region to the centroid, where the conversion plant was assumed to be. If transport was from one region to another, route lengths between 20 random selected points in each region were calculated and averaged. The large difference in the size of the NUTS 3 regions led to a distorted matrix as intra-regional transport was in some cases several times longer than inter-regional transport, which impacted the optimisation. This problem was solved by splitting large NUTS regions to sub-

regions of maximum 7500 km². The feedstock potential was assumed to be evenly distributed in these cases.

2 Methods

Our approach for solving instances of the described problem is simulation-based optimization. We first created a simulation model that calculates costs and several other relevant metrics and has a set of free parameters that can be tuned. The number of different parameters of this model is very large. Therefore, it is infeasible to find optimal parameter settings manually. Instead, we used the simulation model as the objective function for an algorithm that optimizes parameters for the simulation model. Many different algorithms could be used for optimization including exact and inexact solvers. We rely on metaheuristics because we do not need to find a globally optimal solution and we prefer to find approximate solutions in shorter runtimes to iterate quickly. However, it would be very helpful to get accurate information on the best achievable quality. This would be an interesting aspect for future improvements of the method. In the following sections we describe our method in more detail.

2.1 Simulation-Based Optimization

Simulation-based optimization is a term that is used to refer to various different methods (cf. [Spall2003]). We use the term to highlight the fact that simulations are used to determine the quality of a given solution. In this particular problem, a solution is a scenario that describes the value chain including feedstock acquisition, transport and handling, as well as processing, and the quality refers to the overall costs of the solution. The objective is to find a scenario that has minimal overall costs and is potentially profitable. A simulation model is used to try a large number of different scenarios in an iterative loop of simulation and optimization. Figure 3 illustrates this approach. In the center we use an accurate simulation model for evaluating concrete scenarios. This simulation model uses background data such as distance matrices storing the length of transport routes as well regional cost scaling factors and costs for materials and activities. Additionally, the simulation model has several free variables which can be tuned (such as feedstock utilization and transport routes). Through simulation it is possible to calculate detailed measures and results such as plant sizes, transport distances, emissions and most importantly regional costs which can then be aggregated to overall costs (or alternatively a measure describing ROI). Since it is impossible to simulate all possible solutions only a part of the full search space can be explored using some kind of (stochastic) search algorithm. The optimization algorithm uses information gathered through simulation to produce new solution candidates which are again evaluated through simulation. The underlying assumption is that solution candidates that are similar to known good solution candidates also have a similar quality and might be even better. We hope to find improved solutions by iterating this loop many times.

Whether new solution candidates are generated deterministically or stochastically is secondary. Many optimization algorithms in particular meta-heuristics rely on a form of stochastic search. As a consequence of stochastic search the results are also stochastic and multiple restarts of the same algorithm produce different results.

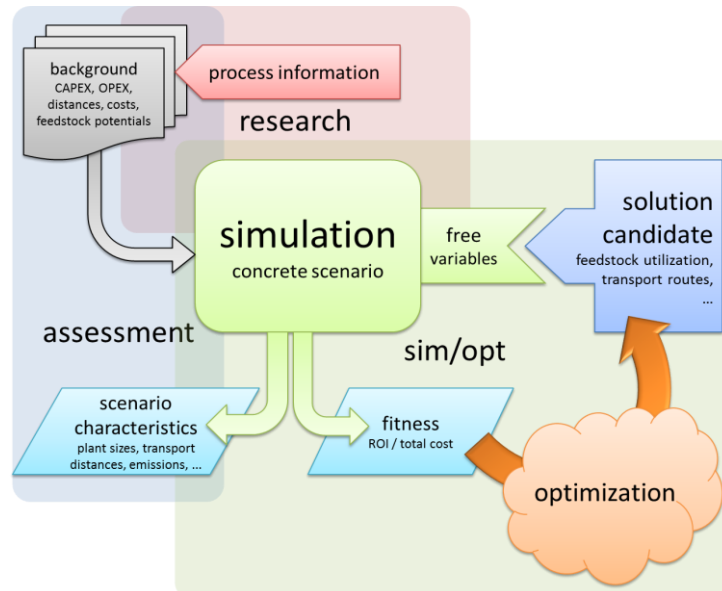


Figure 3: The iterative cycle of simulation-based optimization

Usually, the simulation model itself is also stochastic with the consequence that the simulation results are random variables. In the particular case of the BioBoost problem we decided to implement a deterministic simulation model which produces crisp result values (instead of samples or random distributions) and always produces the same results for the same input values. Therefore, the BioBoost simulation model is actually a rather complex function that can be evaluated efficiently without relying on computationally expansive methods such as Markov Chain-Monte Carlo sampling or discrete event-based simulation. This makes it possible to simulate millions of different scenarios in the optimization step which is necessary to find good solutions.

2.2 Metaheuristics

Optimization problems can be categorized based on their characteristics; most importantly the type of variables, the type of constraints on input variables, and the characteristics of the objective function. This categorization is important because optimization methods can be tuned specifically for problem characteristics. It is often possible to use a standard solver if an optimization problem can be formulated in a way that it matches the characteristics of a certain problem class for which efficient and effective optimization methods have been developed. Examples are real-valued linear programming problems or convex optimization problems which can often be solved efficiently.

Optimization problems stemming from real world applications are often more complex and therefore must be simplified before an efficient standard solver can be applied. A major drawback of simplification is, however, that solutions for the simplified problem might not be optimal for the original problem or might be infeasible. In such cases it is therefore often necessary to implement new variants of optimization methods or to rely on very general solvers which are less efficient but are still able to find solutions to the original problem.

For the BioBoost project we created a complex simulation model to be able to determine accurate and realistic estimates for different scenarios of technology implementation. The model has integer- and real-valued variables and is non-linear in the objective function because of non-linear costs for scaling plants and costs for feedstock. The BioBoost optimization problem can therefore be assigned to the class of mixed integer non-linear programming problems (MINLP).

Meta-heuristics are methods for solving optimization problems that are not specific to a certain problem class [Glover2003]. They only describe the general framework for solution algorithms where certain steps must be adapted specifically to the problem. Many meta-heuristics draw analogies to natural processes. Examples for well-known meta-heuristics are genetic algorithms, evolution strategies, tabu search, and simulated annealing. We performed experiments with different genetic algorithms and evolution strategies and found that a specifically tuned evolution strategy is able to produce comparatively good solutions.

2.2.1 Evolution Strategies

Evolution strategies [Reich1973] (ES) are considered as one of the earliest meta-heuristic and have been developed at around the same time as genetic algorithms (GA). Since their first conception many different variants of ES have been developed. The covariance matrix adaptation evolution strategy (CMA-ES) [Hansen2001] is one of the most well-known variants and particularly effective for many multi-modal and real-valued objective functions. In evolution strategies, solution candidates are encoded as a fixed-length real-valued vector.

ES are population-based algorithms and draw analogies to evolutionary processes in nature. The algorithm starts with a population of random solution candidates. New solution candidates are generated as stochastic variations of random parent solution candidates (mutation). The fitness of all generated individuals is evaluated and only the best solution candidates are kept for the next generation. This process of parent selection, variation and offspring selection is continued until a termination criterion is met. Important parameters of the algorithm are population size μ , the number of offspring produced in each generation λ and whether the new population is selected from parents and offspring (called " $\mu + \lambda$ "), or only from the offspring (called " μ, λ "). In addition to mutation, recombination can be used to create new individuals out of two or more parents.

For the BioBoost problem we implemented an ES variant that uses a mixed encoding of integer and real vectors and uses problem-specific mutation and crossover operators. We

found that variations that stochastically change solutions by changing elements of vectors often produced infeasible solutions. Therefore, we implemented operators that create stochastic variations on a semantic level (e.g. moving plants) and adapt the solution vectors accordingly. These operators proved to be much more effective than simply changing the solution vectors.

3 Results

The implementation is based on the open-source optimization framework HeuristicLab [Wagner2007] and has been developed as a plugin. Both the plugin itself as well as all the data, used to produce these results have been approved by the BioBoost-consortium and are also released as open-source³.

The output of the simulation optimization process is not only optimized choices for locations, feedstock acquisition ratios and transport routes but a plethora of support information, most importantly a per-plant cost breakdown as shown in Figure 4 that, on the one hand, helps to pinpoint the most promising initial locations as well as estimates for further expansion.

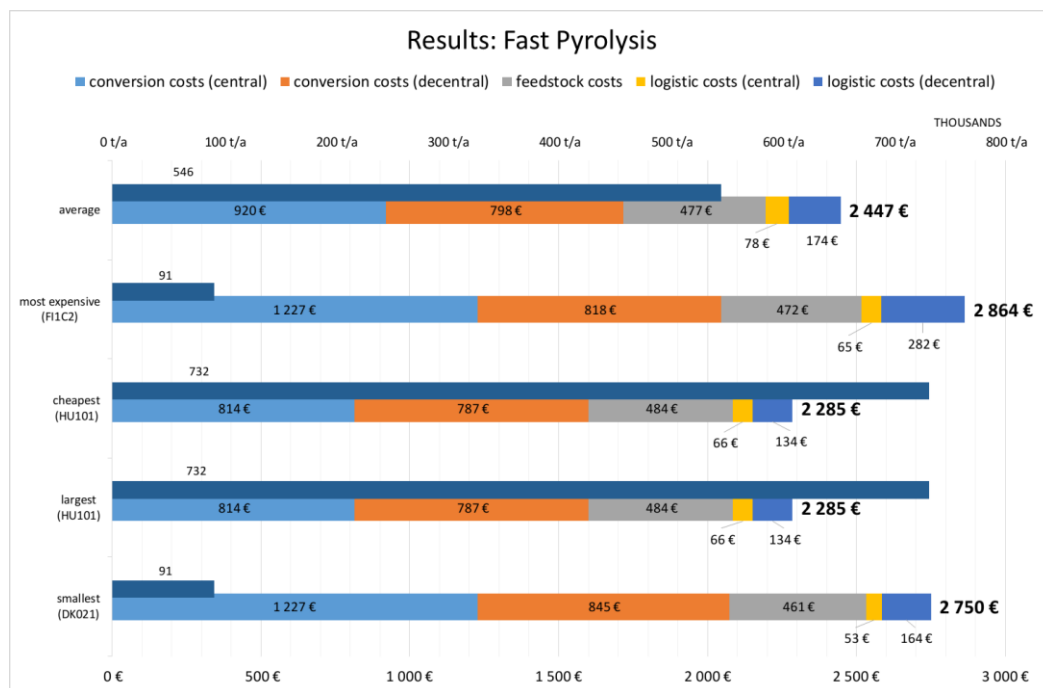


Figure 4 Detailed Results Breakdown

Finally, Figure 5 shows the visualization of transport vector for both feedstock and intermediate energy carrier as well as the production cost of transport fuel per ton encoded in the color palette of the individual regions.

³ <http://dev.heuristiclab.com/>

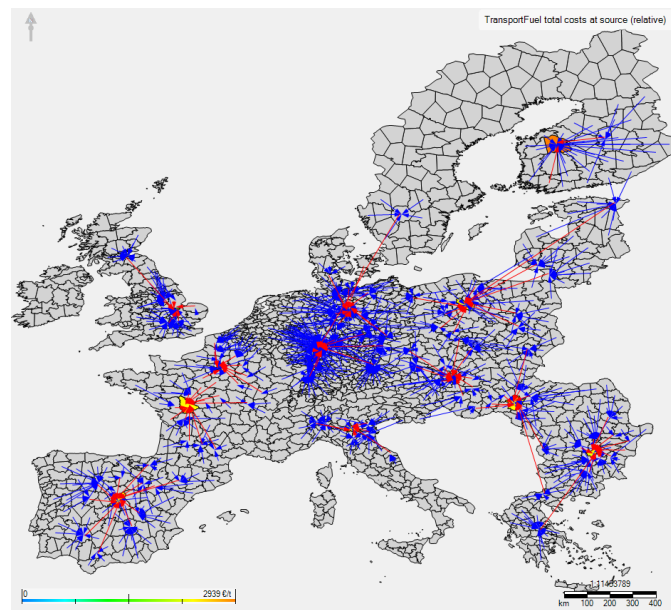


Figure 5 Results Visulationzation on Map

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