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Modeling of Main Material and Energy Flows of a Chemicals Company and LCA of Products thereof

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Abstract

Optimization of mass and energy flows of a chemicals company is an economic and ecologic need. A model of main material and energy flows at Cognis has been developed. The model shows the flows on different levels of complexity. It supports detection of energy and material saving potential, discloses flows of intermediates or end products in the whole company, and supports life cycle assessment (LCA).

Keywords

Oleochemistry, mass balance, energy balance, life cycle assessment

1. Introduction

For years, costs for energy and other raw materials have risen. On the other hand climate change is a challenge to minimize use of fossil resources. Therefore, economic and ecologic demands make it necessary to optimize mass and energy flows in a chemicals company steadily.
Optimization has to be done on all levels of a company, in a process unit, a production plant, the supply chain, the production site or the whole company. As sustainability will be one of the main drivers for innovation in future, the demand for life cycle assessment will rise. Products, which cause less environmental impacts and consume less fossil energy during their life cycle,

have to be developed [1]. Therefore, a model of main material and energy flows at Cognis has been developed.

2. Cognis Oleochemistry

Cognis produces oleochemical derivatives for cosmetics, detergents, cleaners and industrial uses. The chemistry is based mainly on oils and fats from renewable sources, such as coconut oil, palm kernel oil and others. Like in fuel based chemistry a wide variety of products is made from a small base of raw materials.

Oils are split to fatty acids or fatty acid methyl esters and glycerol. Afterwards these base materials are reacted to fatty alcohols, fatty alcohol ethoxilates, sulphated fatty alcohol ethoxilates and many others. Here, reactants from fossil source are used as well. At all stages of production, chemicals are produced for sale as well as used as in-house intermediates for derivatives.

Life cycle assessment has been done at Cognis for more than 15 years. Life cycle inventory data for raw materials and products was published [1-3] and has been used in many life cycle assessment [4 - 6].

3. Development of the Model

3.1. Methodology

Umberto, a commercial software tool for modeling flows, was used to model mass and energy flows on different levels of production. In Umberto no physical or thermodynamic modeling is done, but material and energy balances are calculated from user defined input and output relations. Flow size can be represented in sankey diagrams (fig. 2).

Model data of a dBase based life cycle model of Hirsinger [1-3] was used for a first structure of the company model. Input and output relations are stored in a data base. In the software tool Umberto input and output data can be aggregated on different levels by subnets, which can be stored as units in data base. Thus, scenarios on different levels can be built. For the company model the smallest element for input and output relation is a production unit, such as reaction or distillation. On the second level these units are aggregated as a subnet of the production scheme of a product. Subnet units for the production of a final product can be joined to scenarios for a production site, a business unit, the whole company or for life cycle assessment.

In Umberto squares represent processing units, circles stand for reservoirs (fig.1). All reservoirs can be used on any level of the model.

3.2. Level 1: Esterification

On the lowest level, in detail all energy and material flows are represented in the model. Fig. 1 shows an esterification [7]. Representation is similar to a conventional process flow chart. In addition, Umberto sankey diagrams show flow sizes. Moreover simulation calculations by parameter variation can quickly be done. On the lowest level, the input/output model cannot replace thermodynamic modeling, but it shows which influence on the overall system a reduction or an enhancement of a stream has, or whether recycling of flows is feasible. In this view reservoir heat recycle acts like a market place for heat flows. Heat of a product or water stream run in and can be used again to heat other flows.

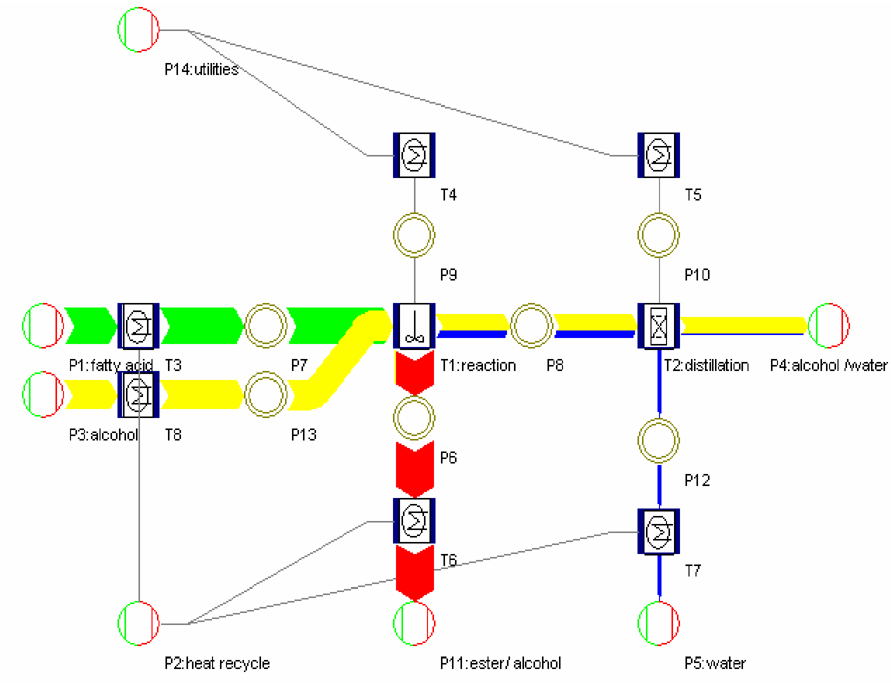

Fig.1: Esterification

3.3. Level 2: Production of fatty alcohol C12/C14

Fig. 2 shows the production of fatty alcohols. Starting from a coconut oil, methyl ester is produced, distilled and afterwards hydrogenated to fatty alcohols, which are distilled to special qualities. Nets like fig. 2 or cutouts from it can be stored as subnets in the library and can be rearranged in other figures on other levels.

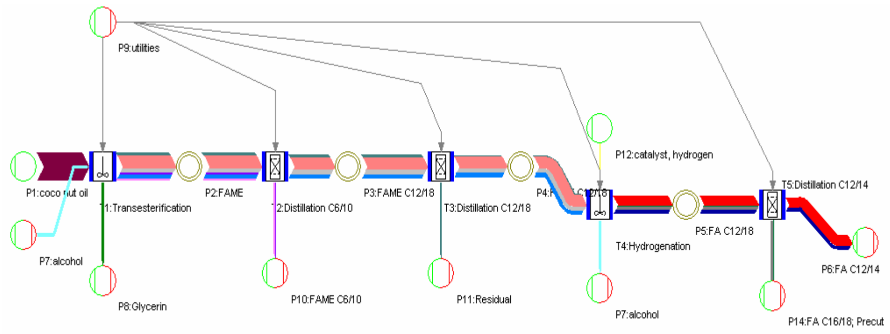

Fig. 2: Fatty alcohol production

3.4. Level 3: Production at Cognis

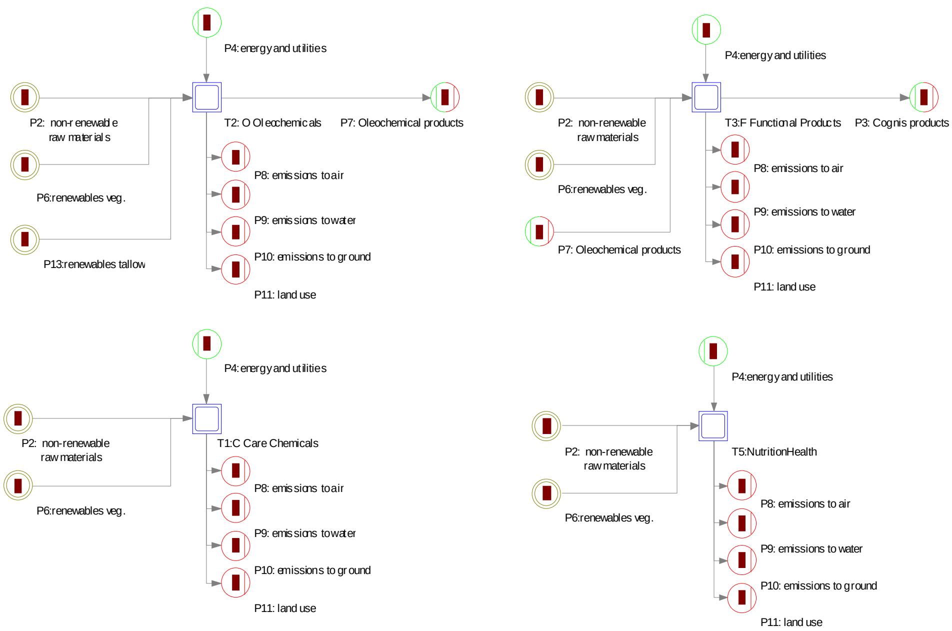

Fig. 3: Model of the company

Fig. 3 demonstrates the production at Cognis. From reservoir renewable resources, oils and fats enter the gate to Cognis and are processed to different products for different business units. Low effort is necessary to rearrange modules from lower levels to other superior levels, e.g. if the structure of the company is changed or if there is a need for an overview of all products of a certain product class, such as esters or ethoxilates.

3.5. Level 4: Life Cycle Inventory from cradle to gate

Fig. 4 shows the production at Cognis as a subnet. All incoming and outgoing materials and energy flows are comprised in this module. Further-on, flows of material and energy in the production of raw materials for Cognis are included. This model supplies information for the life cycle inventory of a life cycle assessment following ISO 14040 [8], ISO 14044 [9]. Moreover, environmental labeling following ISO 14025 [10] will be possible.

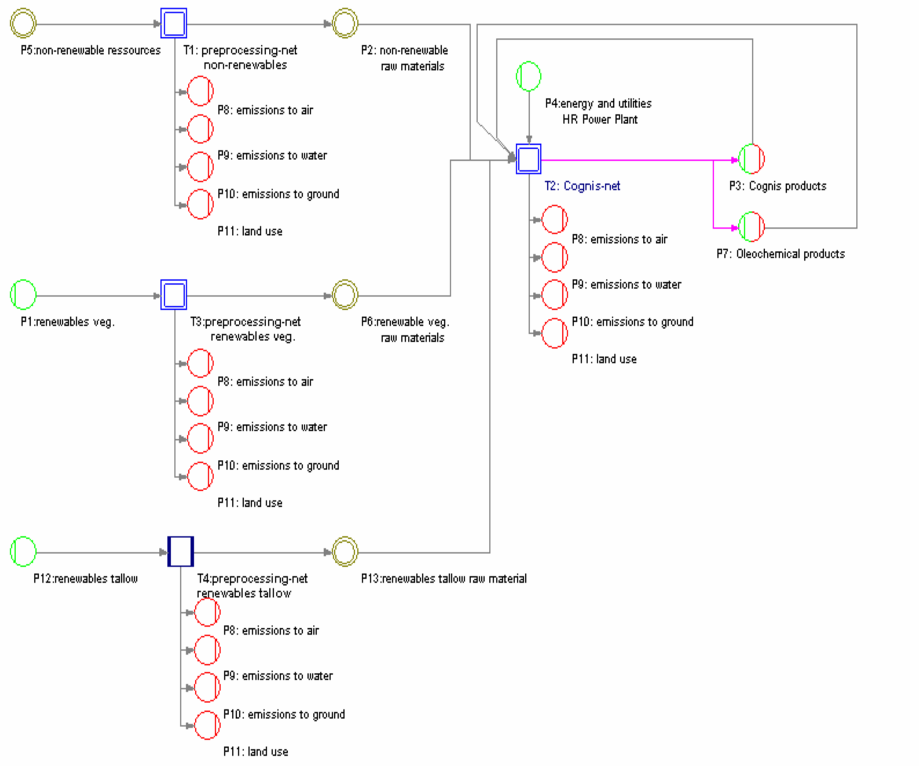

Fig. 4: Net for Life Cycle Inventory

Main flows at Cognis are based on oleochemical raw materials, renewable resources, which do not contribute to global warming. Thus, renewable resources and non-renewable raw materials and the referring processes to produce them are stored in different nets.

4. Conclusions

The Cognis material and energy flow model is capable to fulfill the following tasks:

- Energy and material flows can be retraced on different levels of complexity.
- Detection of energy and material saving potential is supported
- Life cycle inventory for life cycle assessment is part of the model, life cycle impact assessment is supported.
- Environmental labeling is supported.
- The flow of a certain intermediate or end product at Cognis can be retraced.

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