1 Introduction

1.1 Initial Situation and Problem Statement

The substitution of vegetable and animal based raw materials by mineral and synthetic materials was an essential part of the industrial revolution (Tadmor and Gogos, 2006, p. 6). Nowadays, knowledge about the limited availability of crude oil motivates the search for alternative raw materials that can be used to produce industrial goods. In the year 2007, the European Commission identified the market for bio-based products as highly innovative and selected it as a lead market with especially high potential to develop. The establishment of this market is supposed to be very beneficial for economy and society (European Commission, 2007). To become innovation leader, the development of products based on renewable resources is one of the research topics supported by the High-Tech Strategy 2020 of the German Government, which focuses research and innovation activities on selected projects (BMBF, 2010). Renewable resources are of special importance for the chemical industry, since it requires carbon-containing raw materials, which cannot be regenerated otherwise (FNR, 2009).

Renewable resources are defined as "[...] all biomass produced from agriculture and forestry that is not used for food or animal feed" (FNR, 2010). Raw materials are defined as "resources required in the production or processing activity of a firm" (Nahmias, 1997, p. 213). The aim of this work is to develop decision support for supply planning of processors of raw materials from agriculture with customers, who intend their use for the production of physical goods. Non-food applications of renewable resources for the production of physical goods are referred to as material use. If (multiple) material use is followed by energetic use, one speaks of cascading utilization (Oertel, 2007, p. 5). Finding cascading utilization paths and utilizing by-products, which accrue during processing of raw materials, are very important measures to increase resource efficiency (Geldermann, 2012). If renewable materials are used very efficiently, an increasing demand does not necessarily intensify the conflict between the need to use land for food production and for non-food purposes (Carus et al., 2010). Whether material use as the starting point of a cascading utilization path is selected, largely depends on the profitability for the involved companies.

Important agricultural raw materials for material use are sugar cane, corn and potatoes, which supply sugar and starch. Fiber plants like flax, hemp and jute can be used for the production of cellulose while soy, rapeseed and linseed produce oils (Minol and Sinemus, 2004; Carus et al., 2010; Oertel, 2007). In this work, agricultural raw materials are characterized by their seasonal availability, in contrast to other renewable resources that are available throughout the year. Seasonal availability poses an additional challenge for supply planning. Figure 1.1 gives an overview on the energetic and material use of biomass worldwide in 2008, excluding the use of wood. A yearly amount of 175 million tonnes demonstrates the impact of the agricultural sector for the production of physical goods. A detailed analysis of present material use of renewable resources in Germany, Europe and worldwide is given in Raschka and Carus (2012).

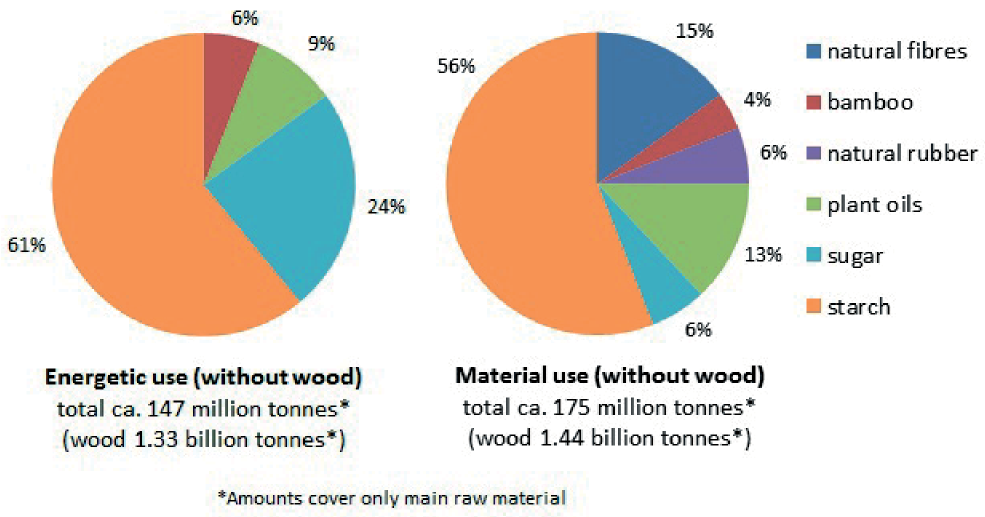

Figure 1.1: Energetic and material use of biomass worldwide 2008 (without wood) (Raschka and Carus, 2012, p. 22)

On macroeconomic level, the generation of added-value and employment through material use is higher than through energetic use (Carus et al., 2010, p. 267). The ability of plants to capture CO_2 implies a positive effect on cultivating and utilizing them to produce goods. The carbon remains stored in the material throughout the lifetime of the product (Oertel, 2007, p. 5). Research is undertaken in agricultural and material science to identify plants and utilization paths that

- result in product properties that are attractive for customers,
- allow for cost-competitive production and
- are environmentally friendly.

These utilization paths will become more attractive if research improves value chains and product properties, extends the areas of application, develops norms and standards and reduces costs (Carus et al., 2010).
In this context, quantitative planning approaches are required for single actors in the supply chain, in order to maximize their profit. The biggest hindrance for market success of bio-based materials is their high price. Bio-plastics are still expensive in comparison to the prices of petrochemical based materials (Lörcks, 2005). Optimized processes might result in lower production costs and motivate material use of renewable resources. The aim of interdisciplinary research should be the optimization of respective production systems and processes, products and raw material supply (FNR, 2009). Presently, quantitative planning approaches for companies in the agricultural sector that consider variability in price, quality and quantity are still a research gap. Ahumada and Villalobos (2009) identify the need to research the design and effect of contracting arrangements for the

particular characteristics of the agricultural market, including policies for buying, selling, delivery and pricing of the products. In particular, they outline a need for stochastic tactical planning models. Geldermann (2012) points out the need to consider specific planning requirements of renewable resources in order to increase resource efficiency.
The agroprocessing industry processes raw materials and intermediate products from the agricultural sector. The Food and Agricultural Organization of the United Nations (FAO) states that “almost all non-food agricultural products require a high degree of processing” (FAO, 1997, p. 222). Some industries are rather active upstream the supply chain and engage in the initial processing of the agricultural commodities as oil pressing, flour milling or saw milling. Downstream industries undertake manufacturing operations on intermediate products as paper production or rubber manufacturing (FAO, 1997, 222 ff). This work focuses on supply planning in upstream agroprocessing industries that process raw materials. The supplied agricultural raw materials originate from farming activities. Farmers might conduct the first processing steps as separation of the grain from the plant and cleansing of grains. Nevertheless, these agricultural raw materials can still show significant quality variations. In this work, examples for agricultural raw materials and their processors is the processing of linseed to linseed oil by an oil mill and the processing of seed by a seed company.
The aim of material use implies specific challenges for supply planning to processors of agricultural raw materials. Industrial customers may wish to ensure sufficient availability as well as stable product quality and price. Processors of agricultural raw materials might be confronted with these requests of customers downstream the supply chain but also need to deal with the characteristics of agricultural production upstream the supply chain. Most of the agricultural crops can only be harvested at certain times of the year. The harvest quality and quantity is uncertain and prices on agricultural commodity markets are subject to variations, too. This situation poses a severe risk to the profit of the processor. Processors play a crucial role in the supply chain of bio-based products as they can reduce quality variations considerably. The development of approaches to efficiently deal with the characteristic challenges of their supply planning decisions might reduce obstacles that keep industrial customers reluctant from using renewable resources.
Planning the supply under several uncertainties and under seasonal availability is a challenge that is not solely restricted to processors of agricultural raw materials for material use. Practitioners from a seed company report a very similar problem, as they need to deal with seasonality and several uncertainties on the supply side as well. Thus, this work deals with two variations of the question how processors of agricultural raw materials should plan their supply. First, decision support is developed for a processor that intends production for an industrial customer aiming at material use. Based on the results, decision support is provided for the seed company.

1.2 Objective and Solution Approach

The aim of this work is to develop decision support for supply planning of processors of agricultural raw materials under consideration of requirements from material use. The processed good needs to satisfy the demand and fulfill the quality specification of an industrial customer. The sales price on the commodity market is uncertain. On the supply side, uncertain supply quality and quantity as well as seasonal availability need to be considered. The decision support should enable practitioners to determine the profit maximizing decisions. Based on the results of this research, decision support for supply planning of a seed company is developed that considers uncertain levels of carry-over inventory, supply quantities and prices on the commodity market as well as seasonal availability of supply.

Stochastic programming provides optimization approaches to deal with uncertain data that can be described through probability distributions. It allows to depict the temporal structure of decisions depending on the availability of information on uncertain values. Stochastic programming can be used to determine decisions that provide flexibility in the face of uncertainty and to maximize the expected profit under simultaneous consideration of all probable realizations of uncertain parameters. Using discrete probability distributions based on available past and present data and the beliefs of the decision maker allows for a decision support that uses all available information and can be applied by practitioners. Modifications of the basic model for material use are implemented to provide decision support for a variety of derived situations.

The structure of this work is oriented at the research objective and the solution approach described before. Due to the variety of products based on agricultural raw materials, the focus in this work is narrowed down on products based on oil crops, though the decision support can be applied to other raw materials as well. In Chapter 2, the composition of plant oils and characteristics of raw material quality are explored. The scope of raw materials and possible reactions with plant oil components is explored in order to provide a detailed understanding of the possibilities for material use. For further investigations on the planning problem of a processor, the oil crop linseed is selected. It is a very promising raw material for the development of new plastic materials. In terms of resource efficiency, it is a very attractive plant as all of its parts can be utilized for the production of physical goods. Information about its growing conditions, possible products and data about uncertain parameters that need to be considered in the supply planning process are derived from literature. This provides an understanding of the technical and agricultural requirements of the environment of the processor, who is an oil mill in this example.

Based on the findings of Chapter 2, a characteristic supply planning decision of a processor of agricultural raw materials for material use is introduced in Chapter 3. This situation is characterized by the demand of an industrial customer of processed goods with specified quality. Supply quality and quantity are uncertain and raw materials are only available seasonally. The sales price on the agricultural commodity market is uncertain as well. Following this outline of the initial problem, the tasks of supply planning and the supply planning process are described in order to locate the function of the decision maker within a company. A definition of uncertainty is provided and literature on sources of supply uncertainty and the mitigation of supply risk is reviewed. Literature on quantitative supply planning approaches is classified according to the applied risk mitigation strategy. Approaches can be grouped into the strategies of keeping safety stock, diversifying sources of supply, hedging with tradeable contracts, especially derivatives, or with real options, especially non-tradeable flexible contracts. The suitability of these approaches to cope with the challenges of the processor is discussed. Characteristics of the structure of agricultural commodity markets are pointed out. The suitability of contract farming and option contracts as hedging instruments in the agricultural sector is discussed. A strategy for the processor to ensure supply continuity is developed. Decision support for the described problem is identified as a research gap.

In Chapter 4, quantitative methods to handle uncertain data are reviewed. Based on the findings in Chapter 2, the availability of data on the uncertain values is systematized and compared to the requirements of several quantitative methods. Stochastic programming is selected as a suitable optimization method to incorporate information on uncertain values that can be described by probability distributions. Based on past data, information about the actual planning situation and expert knowledge, this should be possible for the uncertain values in the decision of the processor. The structure of two-stage stochastic programs with recourse is explained. Formulas are provided to calculate the expected value of perfect information (EVPI) and the value of the stochastic solution (VSS), which are measures for the quality of obtained solutions. Mathematical approaches to find a suitable probability distribution are reviewed. Finally, sensitivity analysis is introduced as a method of post-optimization analysis.

In Chapter 5, the decision situation of the processor is described in detail. Decision support based on stochastic programming is developed. The model is build up step-by-step in order to provide comprehensibility. As it considers a vector of uncertain quality measures, it can be used in a wide area of applications in supply planning for renewable resources irrespective of the specific raw material. The basic model is verified thoroughly by analyzing its decisions in test cases. Modifications of the basic model are presented to depict selling of by-products, penalty costs proportional to the extent of the shortage or a price escalation clause in the objective function. Additionally, the possibility to split optional supply, to sell ordered product to two industrial customers and the presence of two quality grades on the commodity market are depicted in verified models. It is possible to combine some of these extensions, which allows for a large spectrum of possible real-world applications. The set of presented modifications of the basic model clearly shows the adaptability of the optimization approach to different planning situations as a strength of stochastic programming.

Based on the analysis in Chapter 2, realistic data on linseed is used in Chapter 6 to apply the developed decision support to the supply planning problem of an oil mill. A numerical analysis of the basic model and its results is provided by testing different data sets for the commodity market price, calculating the EVPI for all cases as well as calculating solutions with deterministic values and instances with only a single stochastic parameter. A sensitivity analysis for variations of the deterministic values and a worst-case analysis are carried out. A reference case is selected and used to validate the modifications of the basic model. For all modifications, the EVPI solutions with single stochastic parameters and solutions with deterministic values are calculated as well.

A real-world case study on supply planning of a seed company is presented in Chapter 7. It illustrates the relevance of this work for practitioners in the agricultural sector. Investigating the supply planning process of the company provides insights into the state of the art in the agricultural industry and how quantitative planning approaches can support the decision makers in finding the profit maximizing supply plan. The seed company uses stock-keeping instead of optional supply to mitigate supply risk that originates from uncertain purchase price, level of carry-over inventory and supply quantity. The decision

on the required acreage for contract farming is modeled and tested with real-world data, especially with different probability distributions for the uncertain parameters. For the tested cases, the VSS is calculated to estimate the improvement gained in a real-world situation by using stochastic programming instead of an expected value approach.
In Chapter 8, findings of this work are summarized and possible applications of the developed planning approach are described. An outlook on research opportunities concerning the model, the applied methodology and possible further applications of the developed approach conclude this work.

2 Material Use of Agricultural Products from Oil Crops

According to their use, agricultural crops are categorized as food, feed or industrial crops. Industrial crops are mainly grown for the production of industrial goods such as fibers, oils, rubber or pharmaceuticals (Singh, 2010). Due to the variety of products based of agricultural raw materials, the focus in this work is narrowed down on products based on oil crops, which are a subgroup of industrial crops. Figure 2.1 provides the percentage of the most important industrial crops for fiber and oil production on the worldwide material use in the year 2008 (Raschka and Carus, 2012). The total amount of 24 million tonnes of oil plants for material use proves well the importance that these raw materials have already gained by now. Obviously, there is more potential for the future, as crude oil prices increase.

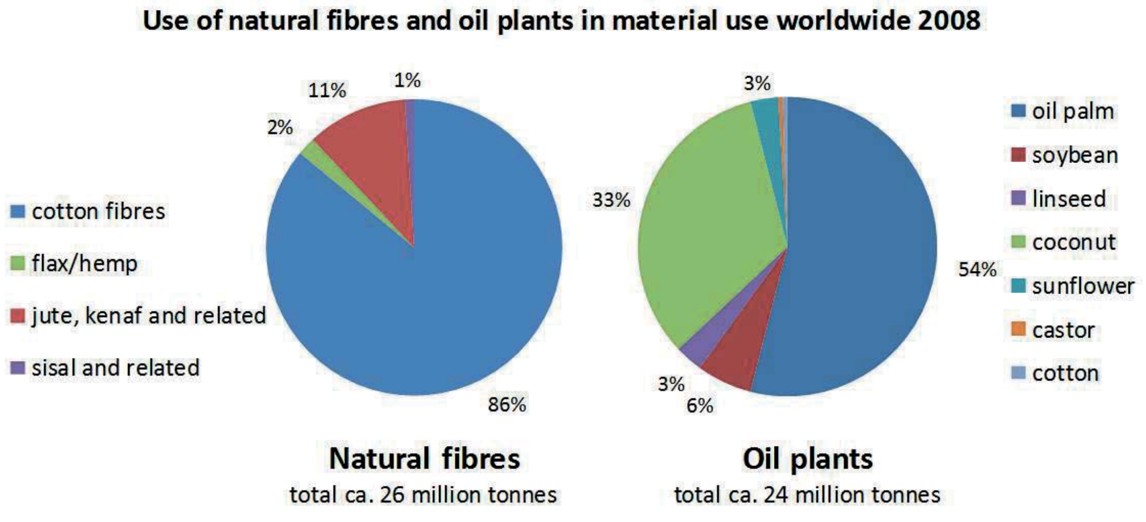

Figure 2.1: Use of natural fibers and oil plants in material use worldwide 2008 (Raschka and Carus, 2012, p. 23)

The seeds of oil crops contain a multitude of substances that can be modified in different reaction paths to create industrial products. Many applications for intermediate products based on oil crops are possible and have been investigated in scientific studies. For most of them, economic data is not available, either because there has not been a scale-up or because information is disclosed. Therefore, the impact and variety of supply planning problems of processors of oil crops can be grasped by understanding basic properties and quality indicators of oils and by gaining an overview on their possible applications as provided in Section 2.1.

Putting the focus of the analysis on one industrial crop allows for congruence of the relevant information and data on price, harvest quality and quantity. To provide a set of realistic data, possible applications based on linseed are presented in Section 2.2. The spectrum of potential usage options is very broad. As the whole plant can be used, linseed utilization paths can be very resource efficient. Figure 2.1 shows the influence of flax for fibers production and linseed for oil production. The term flax usually denotes varieties of linseed with long fibres in the stem. Of special interest is the future use of plant oils as a raw material for the production of plastic materials, which offers plenty of business opportunities.

2.1 Industrial Use of Oil Crops

In the year 2010, the worldwide consumption of vegetable oils was approximately 137 million tonnes. Out of that, approximately 32 million tonnes have been used in the non-food sector e.g. for the generation of energy or in the chemical industry (Fry and Fitton, 2010; ERS, 2012). In the year 2008, the total amount of vegetable oils used in Germany was 5.6 million tonnes and out of that, 1.1 million tonnes were used for technical applications. Approximately 70 % of the oil used for technical applications was imported - mainly palm, soy and coconut oil (Raschka and Carus, 2012). Common areas of application are shown in Table 2.1.

Table 2.1: Areas of application of oils and fats in the chemical industry (see Baumann et al. (1988))

Substance	Application
Fatty acids and derivatives	Plastics; metal soaps; washing and cleaning agents; soaps; cosmetics; alkyd resins; dyestuff; textile, leather and paper industries; rubbers; lubricants
Methyl esters of fatty acids	Cosmetics; washing and cleaning agents
Glycerol and derivatives	Cosmetics; toothpastes; pharmaceuticals; foodstuffs; laquers; plastics; synthetic resins; tobacco; explosives; cellulose processing
Fatty alcohols and derivatives	Washing and cleaning agents; cosmetics; textile, leather and paper industries; mineral oil additives
Fatty amines and derivatives	Fabric conditioners; mining; road-making; biocides; textile and fiber industries; mineral oil additives
Drying oils Neutral oil derivatives	Lacquers; dyestuff; varnishes; linoleum Soaps

2.1.1 Composition of Oils

Plant oils and fats mainly consist of triglycerides, which are esters of glycerol with long chain fatty acids. A schematic illustration is given in Figure 2.2. Triglycerides that are liquid at room temperature are called oils, while triglycerides that are solid at room temperature are called fats. Usually seed oils contain 98 % of triglycerides. Mono- and diglycerides are rather rare in good quality oils, since they are a product of enzymatic activity (Scrimgeour, 2005).

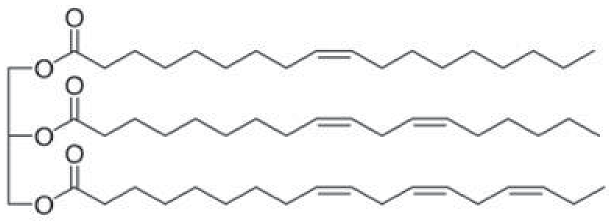

Figure 2.2: Schematic illustration of a triglyceride (Baumann et al., 1988)

Natural fatty acids differ in their lengths and can have different functional groups. Double bonds are the most common functional group beside the carboxyl group. In the short notation for fatty acids, the first number given in brackets indicates the number of carbon atoms in a fatty acid and the second the number of double bonds. Natural oils often contain relevant percentages of the saturated palmitic (C16:0) and stearic (C18:0) fatty acid and of the unsaturated oleic (C18:1), linoleic (C18:2) and linolenic (C18:3) acid (Petrović, 2008). Most natural fatty acids are C4 to C22, with C18 most common. The triglyceride shown in Figure 2.2 is an ester of glycerol and oleic, linoleic and linolenic acid. The fatty acid distribution, as given in Table 2.2 for the most common oils, determines the properties of the oil and its products. Typically, the fatty acid distribution indicates the mass fractions of different fatty acids (Scrimgeour, 2005). Coconut oil and palm kernel oil have a high share of fatty acids with 12 or 14 carbon atoms and are often used for the production of surfactants for washing and cleaning agents or in cosmetics. Linseed, soybean, palm, rapeseed and sunflower oil contain mainly saturated and unsaturated C18 fatty acids. They are attractive raw materials for polymer applications and lubricants (K. Hill, 2000).

The fatty acids distribution of natural oils can vary between genetically different cultivars of the same species or between plants of the same cultivar, which have been exposed to different environmental conditions. Even if two oils have the same fatty acid distribution, there could still be a different distribution of triglycerides, since the fatty acids could have different positions in the molecules. Taking the example of the triglyceride given in Figure 2.2, its spatial structure would depend on the fatty acids in the middle position and in the outer positions. Further, the spatial structure of a triglyceride respective its fatty acids is influenced by the spatial orientation of the double bonds. In *cis*-double bonds, both neighboring endings of the carbon chain are oriented to the same side, which introduces an pronounced bend in the chain. In *trans*-double bonds, they are oriented to opposite sides. Usually the melting points of the *trans*-acids are closer to those of the corresponding saturated fatty acids than to the melting points of the *cis*-acids. Most fatty acids synthesized in plants contain *cis*-double bonds and have even numbers of carbon atoms (Scrimgeour, 2005; Petrović, 2008).

An aggregate measure for the amount of unsaturation, i.e. double bounds, is the iodine value (IV) that indicates the “amount of iodine in g that can react with double bonds

Table 2.2: Typical fatty acid compositions of selected plant oils (in %) (Petrović, 2008).[a]

Carbon atoms: Double bonds	8:0	10:0	12:0	14:0	16:0	16:1	18:0	18:1	18:2	18:3	20:0	20:1	22:0	22:1	24:0	Iodine value	World production[b]
Canola oil				0.1	4.0	0.3	1.8	60.9	21.0	8.8	0.7	1.0	0.3	0.7	0.2	100-115	
Castor oil[c]					2.0		1.0	7.0	3.0							81-91	0.44
Coconut oil	7.1	6.0	47.1	18.5	9.1		2.8	6.8	1.9	0.1	0.1					7-12	3.33
Corn				0.1	10.9	0.2	2.0	25.4	59.6	1.2	0.4		0.1			118-128	2.02
Cottonseed oil			0.1	0.7	21.6	0.6	2.6	18.6	54.4	0.7	0.3		0.2			98-118	3.92
Linseed oil					6.0		4.0	22.0	16.0	52.0	0.5					> 177	0.63
Olive oil					9.0	0.6	2.7	80.3	6.3	0.7	0.4					76-88	2.81
Palm oil			0.1	1.0	44.4	0.2	4.1	39.3	10.0	0.4	0.3		0.1			50-55	28.13
Palm kernel oil	3.3	3.4	48.2	16.2	8.4		2.5	15.3	2.3		0.1	0.1				14-19	3.50
Peanut oil				0.1	11.1	0.2	2.4	46.7	32.0		1.3	1.6	2.9		1.5	84-100	4.81
Rapeseed oil				0.1	3.8	0.3	1.2	18.5	14.5	11.0	0.7	6.6	0.5	41.1	1.0	100-115	13.05
Safflower oil				0.1	6.8	0.1	2.3	12.0	77.7	0.4	0.3	0.1	0.2			140-150	
Safflower oil (high oleic)				0.1	3.6	0.1	5.2	81.5	7.3	0.1	0.4	0.2	1.2		0.3	82-92	
Soybean oil				0.1	10.6	0.1	4.0	23.3	53.7	7.6	0.3		0.3			123-139	31.88
Sunflower oil				0.1	7.0	0.1	4.5	18.7	67.5	0.8	0.4	0.1	0.7			125-140	9.49
Sunflower oil (high oleic)					3.7	0.1	5.4	81.3	9.0		0.4		0.1			81-91	

[a] Some oil compositions may not add to 100 % due to the presence of minor fatty acids.
[b] Figures from 2003/4, production in million metric tonnes
[c] Contains 87 % of OH-bearing ricinoleic acid (C18:1)