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Feasibility of co-producing arabinoxylans and ethanol in a wheat biorefinery

by

MA Mustafa[1,2], N Misailidis[2], F Mateos-Salvador[1, 2], C Du[2],
J Sadhukhan[1] and GM Campbell[2]

[1]Centre for Process Integration,
[2]Satake Centre for Grain Process Engineering,
School of Chemical Engineering and Analytical Science,
The University of Manchester, PO Box 88, Manchester, M60 1QD

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Abstract

The feasibility of extracting arabinoxylans from wheat bran within a wheat biorefinery principally producing ethanol was investigated. Based on this test case, a framework for evaluating opportunities for co-product production and process integration in wheat biorefineries has been established.

Production of bioethanol is increasing rapidly around the world, in order to alleviate pressure on oil supplies and the environmental burden of burning fossil fuels, as well as to increase national energy security and to rejuvenate rural economies. Bioethanol production in the UK, however, has not yet started. It is recognised that in order to make UK bioethanol production economically competitive and commercially feasible, the ethanol must be produced as one of several co-products within a biorefinery. This would allow scope for more integrated, and hence more economical, processes.

As a first step towards co-product processing and the highly integrated biorefinery concept, arabinoxylans appear promising. Arabinoxylans (AX) have several interesting functional properties relevant to food or pharmaceutical use, are present in wheat bran at high levels, and their extraction is facilitated by using ethanol; this latter point immediately suggests scope for economical recovery within a process principally producing bioethanol.

In the current work, a process for extracting food-grade AX was adapted from the literature. Several possible design configurations were created by which bran could be recovered from wheat and AX extraction from the bran integrated with ethanol production from the remaining wheat. Initial conceptual design based on the creation of an Excel spreadsheet was used to evaluate the different designs and select the most suitable for further investigation and optimisation. In parallel, some supporting experimental studies were performed to provide data for process simulation. Two final designs were then simulated using a commercial process simulation package, SuperPro Designer, in order to compare their economic performance with the base case of conventional wheat-to-ethanol-plus-DDGS.

Recovery of wheat bran via pearling was investigated, both as an opportunity to have bran by-pass the main process and enter the DDGS in a dry state, and as a means of obtaining bran for AX extraction. It was concluded that the costs of electricity and of reduced ethanol yield due to starch losses when pearling was employed exceeded the savings in drying costs. As a means of obtaining bran for AX recovery, pearling offers several advantages: it selectively recovers the outer bran layers, which appear to be more highly concentrated in AX, and it minimises starch losses to the bran stream. However, the fine particles produced by pearling may entail handling difficulties during processing, and the functionality of the AX in these outer layers is unknown. Other things being equal, recovery of bran via conventional hammer milling and sieving appeared to offer a cheaper means of producing AX compared with bran recovery using pearling.

Simulation of the integrated process, considering all capital and operating costs, and basing comparisons on a constant return on investment (ROI), indicated that an AX product of 80% purity could be co-produced with ethanol at a cost of around £3.6-4.6 per kg. This is within the range of comparable viscosity-enhancing ingredients used in the food industry, but is towards the top end of the range. In order to establish a market, AX would therefore need to offer some additional functionality. If a market could be created for AX as a food ingredient with a selling price of £6/kg, the ethanol co-produced could be sold at 14% less than in the conventional process, for the same ROI. The research indicates that creating a market for AX is feasible in terms of production costs if the AX is co-produced with ethanol. On this basis, further research is justified to investigate the functionality of AX from different sources and to establish the potential of AX as a food or pharmaceutical ingredient.

Summary

Production of bioethanol is increasing rapidly around the world, in order to alleviate pressure on oil supplies and the environmental burden of burning fossil fuels, as well as to increase national energy security and to rejuvenate rural economies. Production of bioethanol increases the demand for cereals and hence increases their market price and their profitability for growers. Bioethanol production in the UK, however, has not yet started, although several plans to build bioethanol plants are in progress. It is recognised that in order to make UK bioethanol production economically competitive and commercially feasible, the ethanol must be produced as one of several co-products within a biorefinery. This has the benefit of additional revenue streams, and also of greater process complexity which allows scope for more integrated, and hence more economical, processes. Currently Distillers Dried Grain with Solubles (DDGS) is the major co-product of bioethanol production, but this is a relatively unsophisticated and low value product which is likely to lower in value even further as the amount of bioethanol production increases.

Products from biorefineries must compete with oil-derived products. At the same time, biorefineries must be modelled on oil refining operations and must adopt and benefit from ideas developed in oil refining that have made it the efficient operation it is today. The oil refining model of extensive fractionation in order to extract value from every last drop of the barrel of oil must be adapted and adopted for cereal biorefineries. Oil currently benefits from a relatively low raw material price (an advantage that is slowly being eroded), but oil-derived products also benefit from highly efficient, integrated processes that minimise capital and operating costs. Unless cereal biorefineries adopt the same approach of extensive fractionation and effective process integration, they will suffer a double disadvantage against oil refineries and will fail to achieve competitive operation.

Broadly speaking, it is the bran fraction of wheat that is problematic for non-food processing, in terms of representing a large fraction of the raw material but ending up in a low value product. Starch is fermented to ethanol, protein may be recovered, but bran can currently only be burned or sold as animal feed. Adding value to the bran fraction of wheat is necessary in order to enhance the economics of wheat-based biorefineries. Extraction of components of the bran appears to be the most promising route towards producing added-value products.

As a first step towards co-product processing and the multi-product and highly integrated biorefinery concept, arabinoxylans appear promising. Arabinoxylans (AX) have several interesting functional properties (including viscosity enhancement and gel formation, and possibly foam stabilisation and prebiotic activity), are present in wheat bran at high levels, and can be extracted in a process that uses large quantities of ethanol; this latter point immediately suggests scope for efficient and economical recovery within a process principally producing bioethanol. Extraction of AX would also slightly reduce production of DDGS which, in the face of greatly increased bioethanol production capacity, will be increasingly difficult to find markets for. Previous work has suggested the strong potential of AX as a valuable product from wheat bran, but studies have been hindered by the lack of

a commercial source of AX. However, before further research on the production, functionality and possible end-uses of AX can be justified, it needs to be established whether in reality, under plausible scenarios, AX could be produced at a cost sufficiently low that the creation of a market for this product would be feasible.

Much previous work on AX extraction and functionality has been based on maize; our knowledge of wheat-derived AX (sometimes referred to as glucuronoarabinoxylans (GAX) because of the high proportion of glucuronic acid in the AX) is less advanced. Throughout the current work, 'AX' has been used and is intended to indicate wheat-derived arabinoxylans. It is recognised that some of the claims for AX functionality or possible applications relate to maize-derived AX and have not been verified for wheat AX. Again, until the feasibility of producing AX at reasonable cost has been demonstrated, further research into the functional properties and end-uses of wheat-derived AX is difficult to justify.

The objective of the current work was to develop process simulation tools by which to evaluate the potential of co-producing AX in a UK-based biorefinery principally producing ethanol from wheat. The study would indicate whether creating a commercial source of AX appears economically feasible, and therefore whether further research on wheat-derived AX is justified. The tools would also establish the basis for applying process integration in cereal biorefineries, with a view to further developments in the future in which fermentation products other than ethanol are likely to form the core of biorefinery operations.

Pearling (or debranning) is an advanced wheat fractionation technology that has been introduced successfully into traditional flour milling. Given the desirability of a fractionation-value addition model for cereal biorefineries, analogous to oil refineries, the use of pearling in the proposed ethanol-AX plant was investigated. In conventional bioethanol production, the wheat is hammer milled and the entire milled stocks are sent through the liquefaction, saccharification and fermentation stages of the process. The non-fermentable materials (including bran components and protein) pass through the process as essentially inert non-contributors with several undesirable consequences. Their presence requires additional process water in order for process streams to have sufficiently low viscosity for pumping and for heat and mass transfer. This extra water, in addition to its own costs for purchase and waste treatment, increases the size of vessels throughout the process. The water then has to be removed via expensive drying operations. Pearling could be employed to remove some of the bran and send it directly to DDGS, bypassing the wet processing stages. Taking this idea further, the bran removed via pearling could then form the feedstock for an AX extraction section. Both of these opportunities were evaluated in the current work.

For the current work, a process for extracting food-grade AX was specified, based on the work of Maes and Delcour (2001), Hollmann and Lindhauer (2005) and Kwiatkowski *et al.* (2006). The process employs ethanol to wash the bran and to precipitate the extracted AX, and uses alkaline hydrogen peroxide to extract the AX. Four possible design configurations were created, by which bran could be recovered from wheat and AX extraction from the bran integrated with ethanol production from the remaining wheat. Bran was envisaged to be recovered by either pearling, hammer milling or roller milling, and either sent directly to DDGS or to AX extraction. Initial conceptual design based on the creation of an Excel spreadsheet was used to evaluate the different designs and select the most suitable for further investigation and optimisation. In parallel, supporting experimental studies were performed to provide data on AX yields and starch losses, to incorporate into the process simulations. Two final designs were then simulated using a commercial process simulation package, SuperPro Designer V6.0 (Intelligen Inc., USA), in order to compare the economic performance with the base case of conventional wheat-to-ethanol-plus-DDGS. The two designs were based on recovery of 4.4% of the initial wheat as bran, either via pearling, or via hammer milling with sieving to recover large bran particles, and washing of these particles to recover starch prior to AX extraction.

Recovery of wheat bran via pearling was investigated, both as an opportunity to have bran by-pass the main process and enter the DDGS in a dry state, and as a means of obtaining bran for AX extraction. It was concluded that the costs of electricity and of reduced ethanol yield due to starch losses when pearling was employed exceeded the savings in drying costs. This was the case even without considering the additional capital cost of a debranner. Thus pearling would only be of use within an ethanol plant if the bran so obtained were intended for extraction of added-value products, and if this bran gave, for some reason, superior extraction (in terms of yield or product quality) than bran otherwise obtained.

As a means of obtaining bran for AX recovery, pearling offers several advantages: it selectively recovers the outer bran layers, which appear to be more highly concentrated in AX, and it minimises starch losses to the bran stream. However, the fine particles produced by pearling may entail handling difficulties during processing; further experimental work to investigate the handling and processing properties of such bran is required. Other things being equal, recovery of bran via conventional hammer milling and sieving appeared to offer a cheaper means towards production of AX compared with bran recovery using pearling. However, this preliminary conclusion does not take into account the strong possibility that AX extracted from different parts of the wheat kernel differs in its functional properties. It may be that AX from the outer layers has peculiar and desirable functionality; equally, it may prove that it is the inner layers or crease bran that yields superior AX. Further work on the functionality of AXs from different sources is therefore required (where differences could arise from wheat variety, from agronomic practices and environmental conditions, or from the way bran is recovered during processing).

Simulation of the integrated process, considering all capital and operating costs, and basing comparisons on a constant return on investment (ROI) of 17%, was performed. The simulation was based on a plant processing 350,000 tonnes of wheat per annum and producing around 100,000 tonnes of ethanol and 2000 tonnes of AX. The simulation indicated that an AX product of 80% purity could be co-produced with ethanol at a cost of around £3.6-4.6 per kg. This is within the range of comparable viscosity-enhancing ingredients used in the food industry, but is towards the top end of the range. This implies that in order to create a market for this new product, additional functionality beyond simple viscosity enhancement would need to be demonstrated. The high intrinsic viscosity of AX compared with other non-starch polysaccharides, its high water holding capacity and possible foam stabilisation properties may suffice to give the extra benefit; alternatively, suggested prebiotic activity of AX, if confirmed, may allow AX to command a higher price.

The simulation suggested that if a market could be created for AX as a food ingredient with a selling price of around £6/kg, the ethanol co-produced could be sold at 14% less than in the conventional process, for the same ROI. Thus co-production of AX appears to economically feasible, and the additional revenue could allow a reduction in the selling price of ethanol.

Pharmaceutical applications of AX are also possible, which could allow a selling price much greater than the £6/kg suggested, and indeed could make AX production dominate over ethanol in terms of overall value. However, the market for such pharmaceutical products is likely to be much smaller than a potential food market and unlikely to be able to absorb all the AX production capacity of even a modest bioethanol plant. Further costly purification steps would also be required, to meet the specialised needs of such applications. The current work reached its conclusions based on a conservative AX price for a product that could reasonably be expected to achieve a large market volume as a food ingredient.

The research suggests that creating a market for AX is feasible in terms of production costs if the AX is co-produced with ethanol, and that to do so would facilitate the economic production of ethanol. On this basis, further research is justified to investigate the functionality of AX from different sources and to establish the potential of AX as a food or pharmaceutical ingredient. If successful, such research would help in creating the market end of the equation, in terms of demand for such a product, which would then justify the investment in the supply end, in terms of production capability. Research into the functionality of wheat-derived AX is therefore a critically important next step, for the sake of making this promising product and its benefits available, and for the sake of facilitating the introduction of bioethanol production capacity into the UK.

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List of Abbreviations

AEAX	Alkali-extractable arabinoxylans
AX	Arabinoxylan
COP	Cost of Production
DDGS	Distillers Dried Grains with Solubles
DFC	Direct Fixed Costs
GAX	Glucuronoarabinoxylan
ROI	Return on Investment
VOP	Value on Processing
WEAX	Water-extractable arabinoxylans

1. Arabinoxylans – a promising co-product for bioethanol

Production of bioethanol is increasing rapidly around the world, in order to alleviate pressure on oil supplies and the environmental burden of burning fossil fuels, as well as to increase national energy security and to rejuvenate rural economies. Bioethanol production in the UK, however, has not yet started. It is recognised that in order to make UK bioethanol production economically competitive and commercially feasible, the ethanol must be produced as one of several co-products within a biorefinery. This has the benefit of additional revenue streams, and also of greater process complexity which allows scope for more integrated, and hence more economical, processes. Currently Distillers Dried Grain with Solubles (DDGS) is the major co-product of bioethanol production, but this is a relatively unsophisticated and low value product, which is likely to lower in value even further as the amount of bioethanol production increases (although eventually this may be alleviated as cereals for direct use as animal feed are diverted into bioethanol production, such that DDGS then becomes a more dominant component of animal feed).

Increasing oil prices, along with environmental and sustainability concerns, are the drivers for the development of biorefineries. The basis on which the economics of bioethanol production must be evaluated is oil price; as well as being the driver, oil is the competition. Oil refining is also the model by which sustainable alternatives to oil-derived products might be produced. Oil currently benefits from a relatively low raw material price (an advantage that is being eroded), but oil-derived products also benefit from highly efficient, integrated processes that minimise capital and operating costs. Unless cereal biorefineries adopt the same approach of exploiting process integration, they will suffer a double disadvantage against oil refineries and will fail to achieve competitive operation (Campbell *et al.*, 2006).

Scope for efficiencies through sophisticated integration and optimisation is limited in relatively simple processes such as conventional ethanol production from cereals. In addition to the promise of additional revenue, co-product production implies more complex processes, which in turn implies opportunities for cost savings through clever integration. Integration requires complexity, and co-production creates complexity, so co-production and integration are twin opportunities that must go together. By the same token, the greater complexity of cereal biorefineries compared with conventional cereal processes will require more formalised and systematic approaches to design and optimisation than have traditionally been employed.

Broadly speaking, it is the bran fraction of wheat that is problematic for non-food processing, in terms of representing a large fraction of the raw material but ending up in a low value product. Starch is fermented to ethanol, protein may be recovered, but bran can only be burned or sold as animal feed. Adding value to the bran fraction of wheat is necessary in order to enhance the economics of wheat-based biorefineries. Extracting components of the bran appears to be the most feasible route towards producing added-value products.

As a first step towards co-product processing and the multi-product and highly integrated biorefinery concept, arabinoxylans appear promising. Arabinoxylans (AX) have several interesting functional properties (including viscosity enhancement and gel formation, and possibly foam stabilisation and prebiotic activity), are present in wheat bran at high levels, and can be extracted in a process that employs large quantities of ethanol; this latter point immediately suggests scope for efficient and economical recovery within a process principally producing bioethanol. Previous work has suggested the strong potential of AX as a valuable product from wheat bran, but studies have been hindered by the lack of a commercial source of AX. Equally, until it is demonstrated that a commercial source at a reasonable cost would be feasible, such studies are difficult to justify. Thus, before further research on the production, functionality and possible end-uses of AX can be justified, it needs to be established whether in reality, under plausible scenarios, AX could be produced at a cost sufficiently low that the creation of a market for this product would be feasible. The objective of the current work was therefore to develop process simulation tools by which to evaluate the potential of co-producing AX in a UK-based biorefinery principally producing ethanol from wheat.

While pharmaceutical and other non-food applications of AX have been demonstrated, it is likely that an AX product produced would find use firstly in the food industry, as this is likely to be more accommodating of large volumes and low purity than other applications. Although the title and focus of the current work is on creating the conditions that would allow “non-food products” to be produced from wheat, it must be recognised that the co-production paradigm cannot exclude products with potential food uses. To unlock the non-food potential of wheat requires production of co-products; some of these may be products intended for direct use within the food industry. In the current work, the non-food product of interest is ethanol, and the most promising co-product appears to be AX. This happens to have potential for both food and non-food applications – and the food applications are probably easier to realise in the shorter term. Alternative biorefinery scenarios might have plastics or chemicals such as succinic acid as the major non-food product. Ethanol biorefineries are a stepping stone towards other wheat biorefineries, and integration with food-related products is equally a strategic necessity.

This report describes work carried out to investigate the potential for co-production of AX within a biorefinery principally producing ethanol. Chapter 2 describes conventional bioethanol production and presents the preliminary conceptual design activities by which several process options were evaluated, from which two were selected for further investigation. It presents the four flowsheets initially identified as being plausible alternatives, and describes the Excel-based software tool developed for their preliminary evaluation, leading to identification of two options for full simulation. Chapter 3 presents the conceptual design stage and analyses based on these initial flowsheets, identifying the best candidates for further analysis and full simulation. Chapter 4 presents experimental work carried out in support of the simulation studies, to generate information regarding the distribution of AX within bran layers, and to investigate starch recovery following washing of bran. Chapter 5 presents the detailed simulation of the two options identified in Chapter 3, leading to conclusions regarding the opportunity for extracting AX as a co-product of ethanol production from wheat.

2. Flowsheets for integrated ethanol and arabinoxylan production

2.1 Introduction

In order to produce products that can compete with oil-derived products, cereal biorefineries must adopt the pattern of extensive fractionation and value addition within highly integrated processes than are used by oil refineries. Bioethanol production is ushering in the new world of cereal biorefineries – the need for bioethanol is the driver for developments in this area, but these developments will lead to other products from cereals, including platform chemicals and plastics (Koutinas *et al.*, 2006). For its own sake, and for the sake of the wider range of sustainable products that will follow, there is an urgency for UK bioethanol production to achieve competitive operation as quickly as possible. Adopting the process integration approaches of the oil refining and wider chemical processing industries will play a key role in achieving this early economic operation.

In the case of bioethanol, arabinoxylans (AX) immediately present themselves as suitable candidates for co-production. AX is present in wheat at a high level and has several interesting functional properties that promise valuable applications in both the food and the non-food industries. These properties include viscosity enhancement and gel formation, and possibly foam stabilisation and prebiotic activity (Schooneveld-Bergmans *et al.*, 1999; Bergmans *et al.*, 1996; Courtin and Delcour, 2002; Grootaert *et al.*, 2007). Applications include possible use in bakery and dairy products, incorporation into packaging films and for pharmaceutical products including wound dressings (Courtin and Delcour, 2002; Miraftab *et al.*, 2003; Peroval *et al.*, 2004; Grootaert *et al.*, 2007). In addition, the AX extraction process uses large quantities of ethanol to wash the bran and to precipitate the AX, which immediately offers scope for cost savings through process integration. However, AX is not currently available commercially in large quantities, and some of these applications are not yet demonstrated, particularly for wheat-derived AX. Creation of a commercial source of AX through co-production with ethanol would need concurrent creation of suitable markets for this novel product.

This chapter describes the initial identification of process flowsheets by which bran might be recovered from wheat for the purposes of AX extraction, with the extraction section integrated with ethanol produced in the starch fermentation section. Conventional bioethanol production is described, followed by processes reported in the literature for extraction of AX from wheat bran. The flowsheets developed in the current work to integrate these two activities are then presented. An Excel-based software tool is described that was developed in order to perform comparative calculations of operating costs for the four flowsheets and to undertake sensitivity analyses. The conclusions from these analyses are then presented. The Excel spreadsheet is designed to be suitable for general use (not requiring specialist simulation software and competence in using such software), but does not consider all capital and operating costs. It was used only for initial design consideration and comparison. Full simulations of the most suitable designs identified by this initial activity are presented in Chapter 5.

2.2 Conventional bioethanol production

The bulk of global production of ethanol comes from agricultural alcohol which may be distilled from a number of sources such as grain, molasses, fruit, wine, and cellulose. Roughly 60% of the world's ethanol production is from sugar crops (Berg, 2003). Most of the remainder comes from grain, predominantly from maize, but with wheat becoming increasingly attractive as an alternative feedstock to maize in areas where wheat dominates, such as Canada (Zeman N, 2006). Synthetic alcohol derived from crude oil, gas or coal plays a minor role, accounting for 7% of the global overall output according to Berg in 2003, and almost certainly a lower percentage now, with the recent rapid increase in global bioethanol production capacity.

The conventional production of ethanol from grain goes through a number of stages to produce ethanol and other co-products. The key operations are starch hydrolysis, fermentation and ethanol recovery. Starch hydrolysis is a mature technology that utilises enzymatic liquefaction and saccharification to produce a relatively clean glucose stream, which is then fermented by yeast to produce ethanol. Distillers Dried Grains with Solubles (DDGS) and CO_2 are the main by-products. Figure 2.1 shows a schematic of conventional bioethanol production from grain.

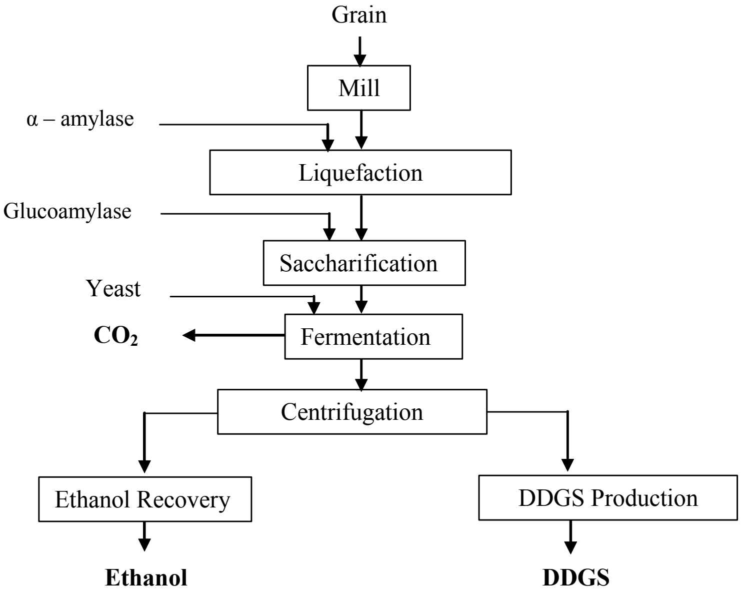


Figure 2.1. Schematic of conventional bioethanol production from grain.

2.2.1 Milling

To facilitate starch extraction and fermentation, grain (usually maize) is initially milled. Two processes may be used for milling. The first, wet milling, is based on soaking the grain in sulphur dioxide at 48-52°C for about 30-50 h. Following the soaking (steeping) of the grain, the soft grain is ground in order to separate the germ from the starch. The germ is washed to free the attached starch and used to produce oil. The starch fraction is further ground and the bran is separated from the starch and protein. The protein is separated from the starch to produce a protein fraction and a starch fraction (Ladisch *et al.*, 1991).

The second milling process, termed “dry milling”, is the most widely used method in the USA for the fermentation of ethanol from grain (Kwiatkowski *et al.*, 2006). Dry milling involves the milling of the whole grain without separation of its components. This provides a much simpler process, and would probably prove to be the most appropriate approach for ethanol production from wheat. Comparing the two methods, although the utilisation of the starch streams through wet milling is more efficient, it is also more complex than dry milling (Ladisch *et al.*, 1991).

Wheat milling for food use employs dry processing. Traditional millstones were replaced in the late 1800s with the introduction of roller milling technology and the gradual reduction process, to give highly efficient separation of bran and endosperm and recovery of white flour (Campbell, 2007). Recently a new wheat milling technology, pearling (or debranning) has been commercialised; adapted from rice milling, this approach uses friction and abrasion to partially remove the outer layers of the wheat kernel. The several benefits of this new technology include superior bread quality, such that the technology has been rapidly adopted by UK flour millers. As an advanced fractionation technology, and with the experience now gained through industrial flour milling applications, pearling potentially has a strong role to play in cereal biorefineries for non-food products. Pearling is already widely used in the USA for bioethanol production from maize (M Clare, personal communication).

Wheat flour mills operate at 70-80% grain to flour conversion efficiency. The remaining 20-30% comprises predominantly bran as well as small amounts of germ and flour. Industrial wheat bran usually accounts for 14-19% of the grain and consists mainly of starch, protein, glucuronoarabinoxylans, cellulose, β-glucan, and lignin (Maes and Delcour, 2001, 2002). It has potential for further processing to create additional co-products to contribute to the biorefinery economics. Bran for further processing in a biorefinery could be recovered from wheat in several ways, including conventional roller milling (with several milling and sifting stages), debranning, or by simple hammer milling followed by sieving to recover coarse bran particles (with adhering endosperm). The different approaches will give brans of different composition and handling properties. In all cases, minimisation of starch losses to the fermentation section would be a key consideration. In current bioethanol operations, all of the wheat is hammer milled and the entire milled stocks sent for fermentation, in order to ensure no loss of starch for conversion to ethanol. Separation of bran for alternative processing would need to be performed in such a way as to minimise any impact on ethanol yield.

2.2.2 Liquefaction

During liquefaction, starch is hydrolysed through the addition of α-amylase to begin breakdown of the starch polymer into soluble dextrins. The process starts by mixing the milled grain with water to form a mash which is transferred to a pre-cooker. This is then sent to a mash heater and cooked at a high temperature of 140-180°C. The mash is then flashed to atmospheric pressure and cooled to 40°C (Lin and Tanaka, 2006).

2.2.3 Saccharification

After the liquefaction of starch, the sugars are mainly in the form of dextrins which still need to be broken down by saccharifying enzymes to sugar molecules of three units or less (Warren *et al.*, 1994). The liquefied starch is hence further hydrolysed using glucoamylase, which converts it into glucose.

2.2.4 Fermentation

The glucose from the previous step is fermented to ethanol using yeast (*Saccharomyces cerevisiae*), with CO_2 as a co-product. The ethanol concentration produced by fermentation ranges from a few per cent up to 14% (Berg, 2003). The temperature during this operation is controlled at 30°C by continuous cooling, as the conversion of glucose to ethanol produces heat. The mode of operation can be continuous or batch; however, continuous operation is favoured since it results in savings in capital cost (smaller fermenters) and an increase in productivity.

2.2.5 Centrifugation

The fermentation step is followed by centrifugation for solid-liquid separation. The products from this step are further processed for the recovery of ethanol and for the production of Distillers Dried Grains with Solubles (DDGS). However, practice with respect to this stage varies. Keim and Venkatasubramanian (1989) show a variation to this step in that the stream resulting from the fermentation step goes through a distillation (ethanol recovery) step prior to centrifugation to yield wet grain and thin stillage, so that no ethanol is lost in the wet solids streams. The thin stillage is further evaporated to yield syrup which is added to the wet solids before dehydration.

2.2.6 Ethanol recovery

Ethanol is recovered using distillation and dehydration. Firstly, distillation renders a product of up to 95.6% ethanol in water (at this point an azeotrope forms and further purification by distillation is not possible). This type of ethanol is called hydrous alcohol. Secondly, a dehydration column removes the residual water by using an entrainer such as cyclohexane, benzene, or pentane. Finally, an ethanol and entrainer-recovery column is used. Other techniques such as molecular sieving are also used to produce very pure anhydrous (water-free) alcohol. 1% gasoline is added as a denaturant such that the final product becomes unfit for human consumption (Warren *et al.*, 1994).

2.2.7 DDGS production

The remaining solids from the centrifugation step are further dried using a rotary drum dryer to produce Dried Distillers Grains with Solubles (DDGS). DDGS is mainly used as an animal feed, however it could also be burned to provide a source of combined heat and power for biorefineries. The final product contains around 9% moisture (McAloon *et al.*, 2000).

2.3 Arabinoxylan extraction

Wheat-based biorefineries are in principle capable of producing a wide range of products, including biofuels, platform chemicals and biodegradable plastics through starch exploitation. However, to boost the biorefinery economics, bran fraction exploitation is also required. The most promising product from bran seems to be arabinoxylan. Schooneveld-Bergmans *et al.* (1999) reported how arabinoxylans could be used as viscosity enhancers, emulsion or foam stabilisers, water absorbents, thickeners, gelling or filling agents and fat replacers. Furthermore, other functional properties of AX, such as their ability to stabilise protein foams and their applicability as a source for the production of oligosaccharides, might offer physiological benefits (Bergmans *et al.*, 1996).

The literature contains a number of proposed procedures for the extraction of AX including work by Bergmans *et al.* (1996), Bataillon *et al.* (1998), Maes and Delcour (2001) and Weightman *et al.* (2002). For the current work, the alkaline hydrogen peroxide extraction and ethanol precipitation procedure proposed by Hollmann and Lindhauer (2005) was selected based on the following considerations:

- It employs inherently low toxicity chemicals, whereas some other procedures use materials inappropriate for a product intended for food use, such as barium hydroxide for the AX extraction instead of alkaline hydrogen peroxide;
- It allows direct bioethanol integration;
- It describes a pilot-scale procedure whereas others are at a lab-scale;
- It provides a relatively high recovery of AX of approximately 50%.

Hydrogen peroxide under alkaline conditions operates by oxidising the lignin in the bran, thereby breaking linkages with the polysaccharides (*i.e.* the AX) and facilitating the latter's extraction (Gould and Freer, 1990; Maes and Delcour, 2001). Maes and Delcour (2001) and Hollmann and Lindhauer (2005) used sodium hydroxide to maintain alkaline conditions; however, NaOH absorbs CO_2 from the air to form carbonates, such that the pH reduces over time. Alternative sources of alkali such as potassium or calcium hydroxide might prove less problematic (Richard Weightman, personal communication).

The AX extraction procedure was modified to be suitable for industrial scale operation as follows:

- Removing the intermediate drying step that was evidently employed for convenience of laboratory operation, but would not be employed at industrial scale;
- Using rotary drum dryers instead of circulating air dryers, to allow ethanol recovery;
- Combining the decantation and centrifugation steps, to simplify the flowsheet;
- Omitting the acetone washing, dialysis and freeze drying steps, since they are suitable for laboratory work but generally inappropriate at the industrial scale.

The slightly modified extraction procedure proposed by Hollmann and Lindhauer (2005) for achieving a 70% purity product is shown in Figure 2.2. Bran is treated (Treatment 1) to remove low molecular weight contaminations and to inactivate arabinoxylan-degrading enzymes. This is achieved by suspending bran in 70% ethanol and heating to 80°C for 4 h with stirring. The resulting slurry is then sieved and washed with 70% ethanol. A second treatment step (Treatment 2) is applied to remove water-extractable arabinoxylan by suspending the purified bran in water for 2 h at 40°C. Once more, the product goes through a sieving and washing step, however this time with cold water. The product from the previous step is added to Treatment 3 which achieves the AX extraction through addition of hydrogen peroxide, pH adjustment to 11, temperature adjustment, and the addition of protein-degrading enzyme (alcalase). This is followed by sieving and washing with water. The collected filtrate is concentrated to one-fifth of its initial volume using an ultrafiltration step. Ethanol precipitation is undertaken using 96% ethanol to bring the retentate to a final concentration to 65%. The precipitated material is allowed to settle out at 4°C. Centrifugation, washing (with 96% ethanol), and drying then follow. This proposed procedure is capable of producing a 70% purity product.

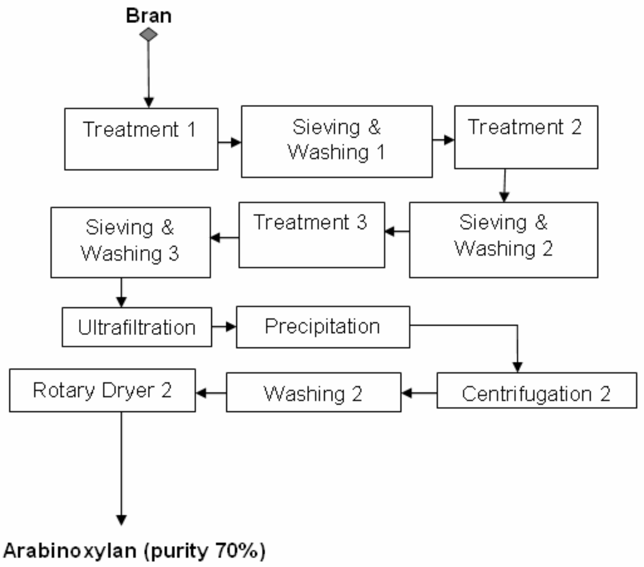


Figure 2.2. Arabinoxylan extraction procedure for achieving a 70% purity arabinoxylan product. The procedure is modified from Hollmann and Lindhauer (2005).

To produce a higher purity product of 80%, β-glucans are removed through an additional purification operation in which an enzyme (lichenase) is added, as shown in Figure 2.3. The additional operation – Treatment 4 – includes the following steps: addition of enzymes, temperature adjustment, pH adjustment, and heat inactivation of the enzymes.

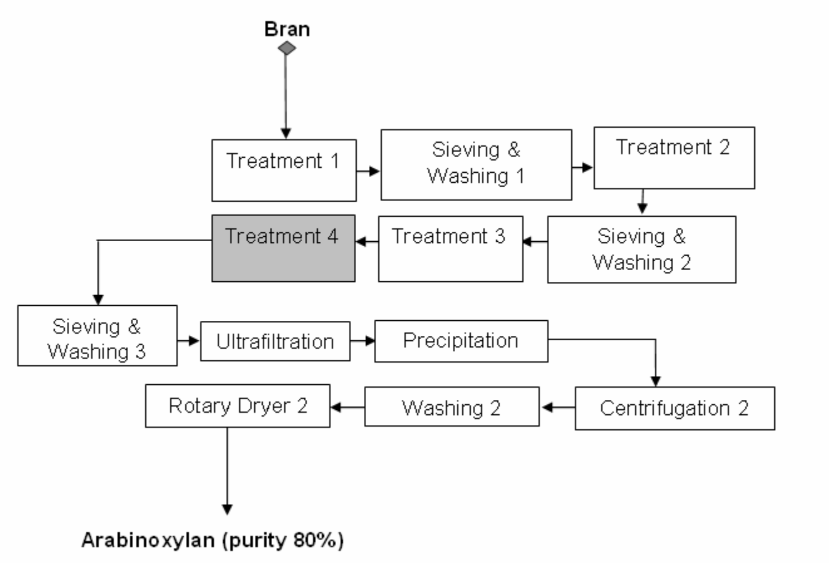


Figure 2.3. Increasing arabinoxylan purity to 80% through the addition of an extra treatment step (Treatment 4) for the removal of β-glucans.

2.4 Initial proposed flowsheets

Four flowsheets were proposed for initial consideration, in consultation with Green Spirit Fuel Ltd., and Satake Corporation UK Division. These flowsheets included:

- The base case of conventional wheat-to-ethanol-plus-DDGS;
- A flowsheet showing recovery of bran by pearling, with the bran being sent straight to DDGS and bypassing the fermentation stage; and
- Two flowsheets including AX extraction but varying in the means of obtaining the bran for this extraction.

The four flowsheets were analysed to investigate the impact of the production of co-products and the employment of the Value Analysis process integration approach (Sadhukhan *et al.*, 2003, 2004; Sadhukhan and Smith, 2006). Based in this work and the results of experimental investigations presented in the Chapter 4, full simulations were performed on two revised AX-extraction flowsheets in comparison with the base case.

2.4.1 Flowsheet 1: Conventional bioethanol production (base case)

Figure 2.4 shows a conventional flowsheet with ethanol as the main product and co-products DDGS and CO_2. The process is assumed to operate in continuous mode and processes annually 340,000 t of wheat. Furthermore, a CO_2 recovery unit is assumed.

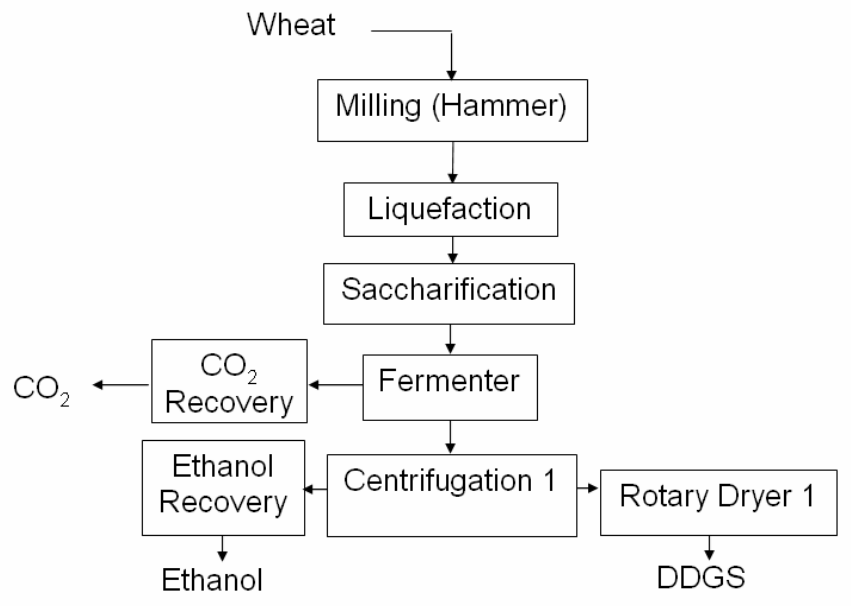


Figure 2.4. Flowsheet 1 – Conventional bioethanol production.

2.4.2 Flowsheet 2: Debranning and sending bran to DDGS

Figure 2.5 shows the introduction of a debranning step prior to the hammer mill. This could allow a decrease in utility consumption through reducing the amount of water required in the process and hence reducing steam consumption for later drying and ethanol recovery steps. On the other hand, this needs to be weighed against the losses of starch in the bran (which translate into ethanol losses), the added capital cost of a debranner, and the increase in electricity consumption for debranning.

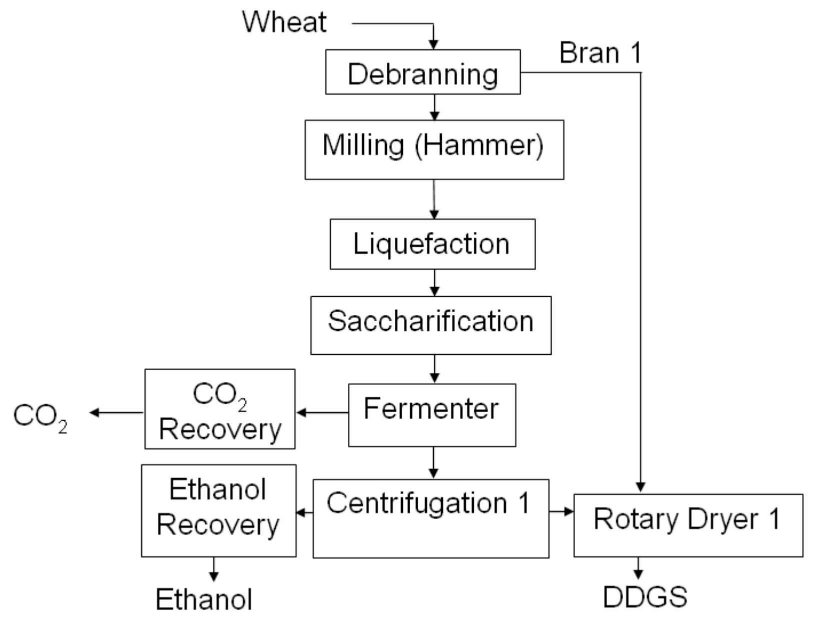


Figure 2.5. Flowsheet 2 – Debranning and sending bran to DDGS.

2.4.3 Flowsheet 3: Sending bran to DDGS and to arabinoxylan extraction

Figure 2.6 expands the previous flowsheet (Figure 2.5) to include an AX-extraction process. The hammer mill is replaced by a debranner and a roller mill system (in practice this would require several roller milling and sifting operations to recover relatively clean bran). The bran stream (Bran 1) is sent to DDGS, whereas a second stream (Bran 2) is sent to AX extraction. Starch from Bran 2 is recovered through a washing step (Washing 1) prior to AX extraction. This configuration could benefit from economic gains in two ways: by sending bran to DDGS, and through the production of a co-product. The rationale of this arrangement, at the time, was that it may have proved to be the case that the bran recovered by pearling was low in AX and unsuitable for extraction, but suitable for bypassing to DDGS, with the inner layers of AX-rich bran then recovered by roller milling. In the end, as the Chapter 4 reports, AX appears to be more concentrated in the outer layers. Thus Bran 1 would probably be better sent for AX extraction than diverted straight to DDGS.

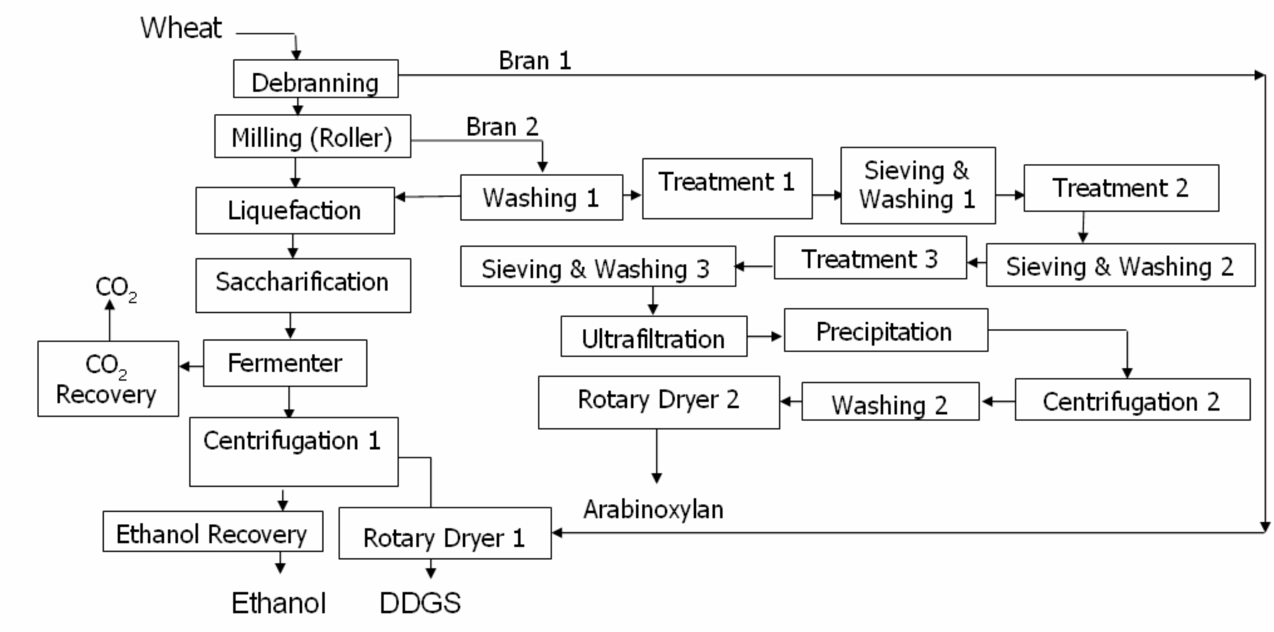


Figure 2.6. Flowsheet 3 – Sending Bran to DDGS and to AX extraction.

2.4.4 Flowsheet 4: Sending all the bran to arabinoxylan extraction

Finally, it is proposed to send all the removed bran to AX extraction, rather than sending any directly to DDGS, as shown in Figure 2.7. This flowsheet retains the flexibility of employing either debranning or roller milling or both to obtain the bran for extraction. It does not imply that all of the bran initially associated with the wheat would be recovered for AX extraction – only that all of the bran recovered would be processed for AX rather than diverted directly to DDGS. It is unlikely in any ethanol-AX co-production facility that all of the bran would be processed and all of the AX extracted, as the market for AX is likely to be much smaller than the corresponding market for bioethanol.

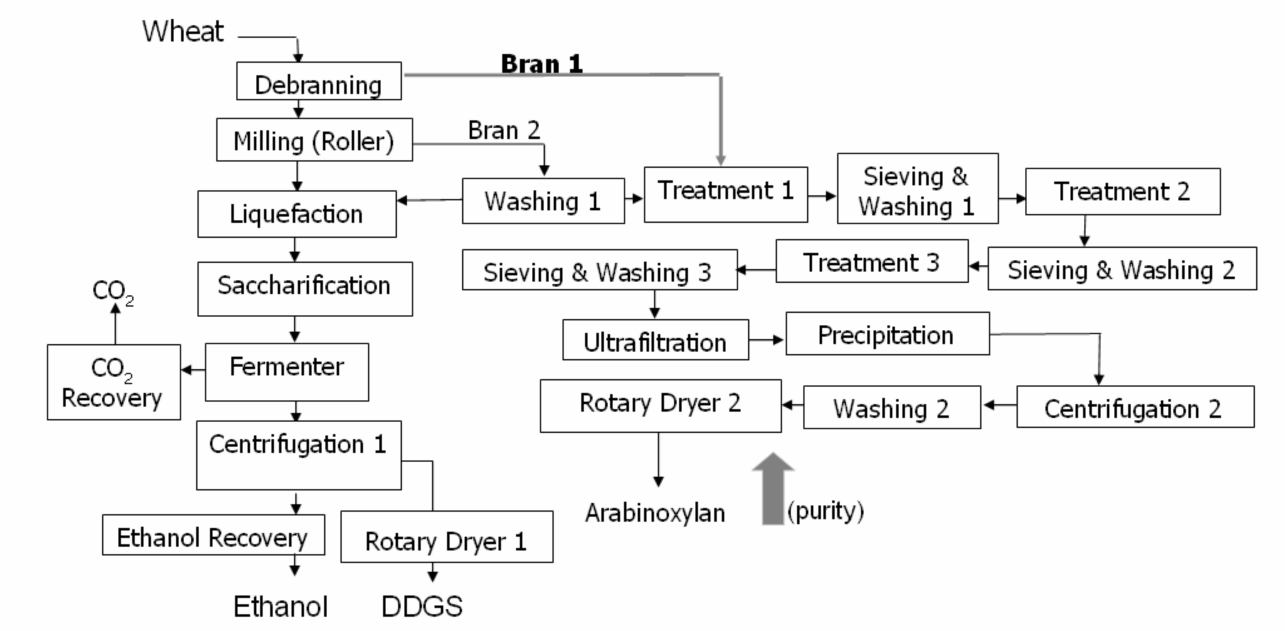


Figure 2.7. Flowsheet 4 – Sending all bran to arabinoxylan extraction.

Figure 2.8 shows a superstructure containing all previous proposed flowsheets and highlighting the starch and bran processing sections. The numbers 1-4 refer to the alternative routes taken within the various flowsheets.

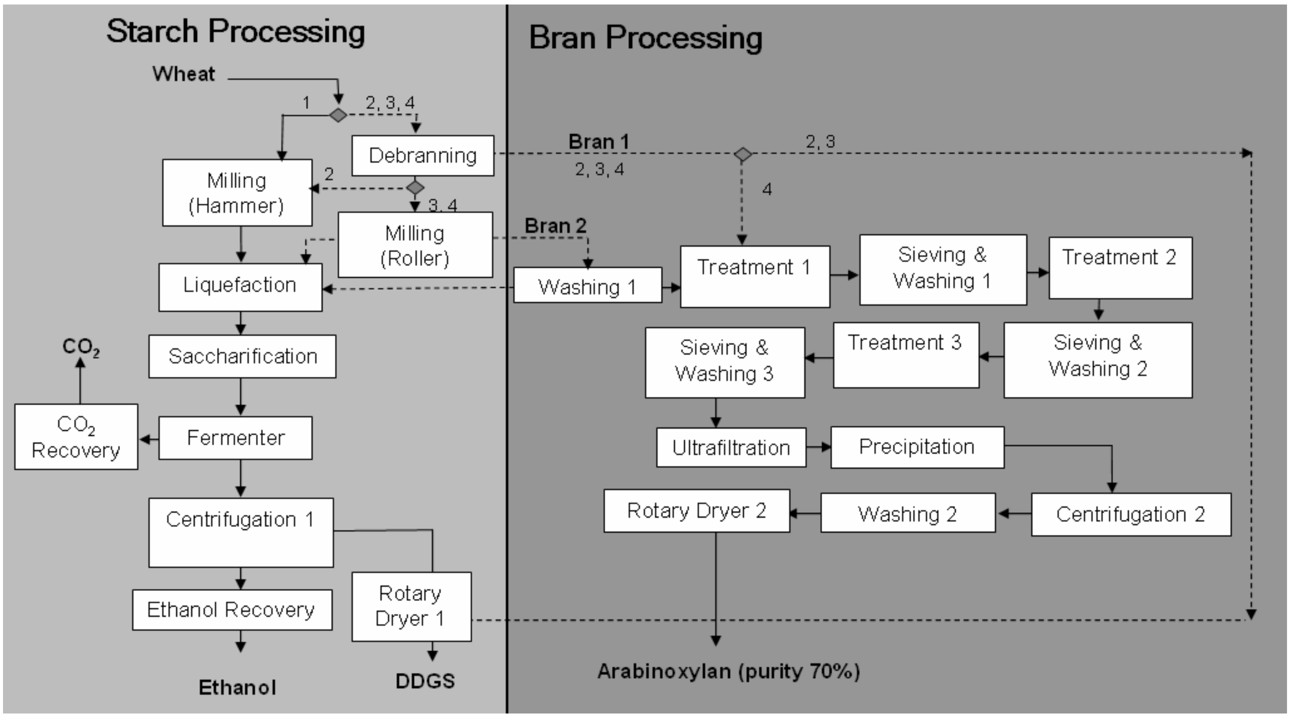


Figure 2.8. Superstructure showing all proposed flowsheets.

Figure 2.9 shows the different raw material requirements for each of the unit operations within the superstructure. In particular, the ethanol concentration required at the various washing and treatment stages is specified. Figure 2.10 shows the different utility requirements for each of the unit operations within the superstructure.

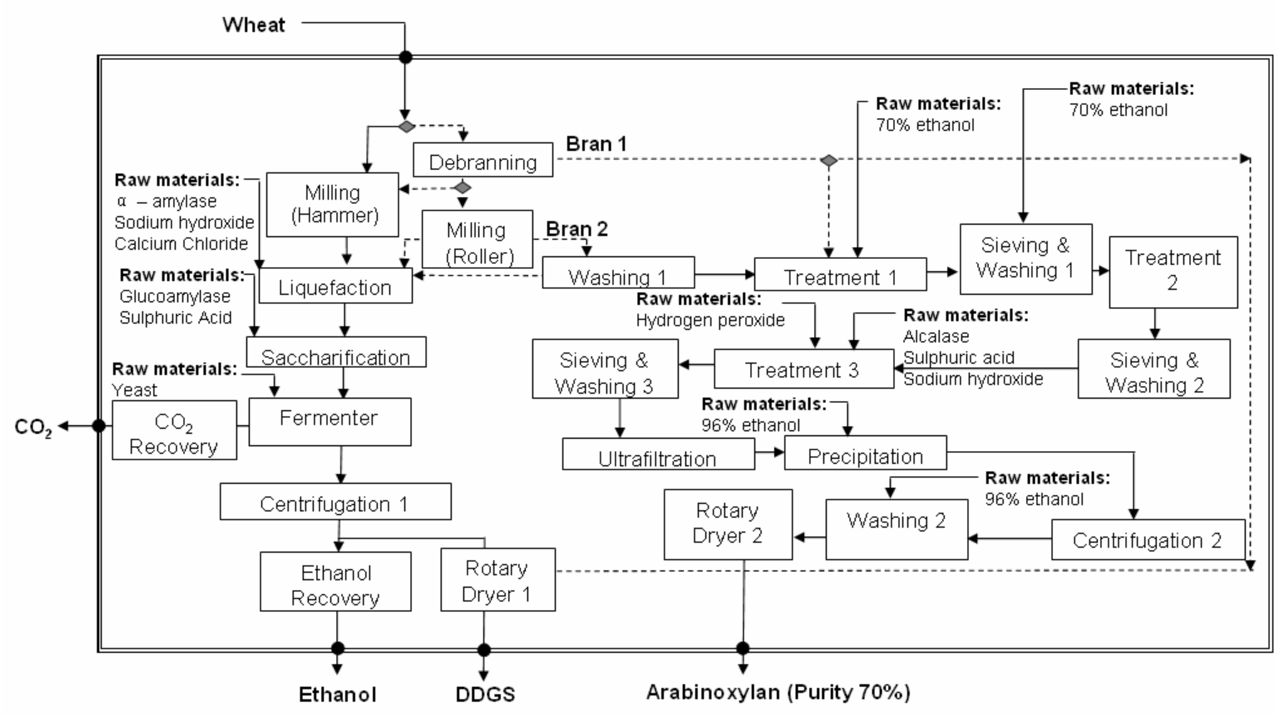


Figure 2.9. Superstructure showing all raw material requirements for the proposed flowsheets.

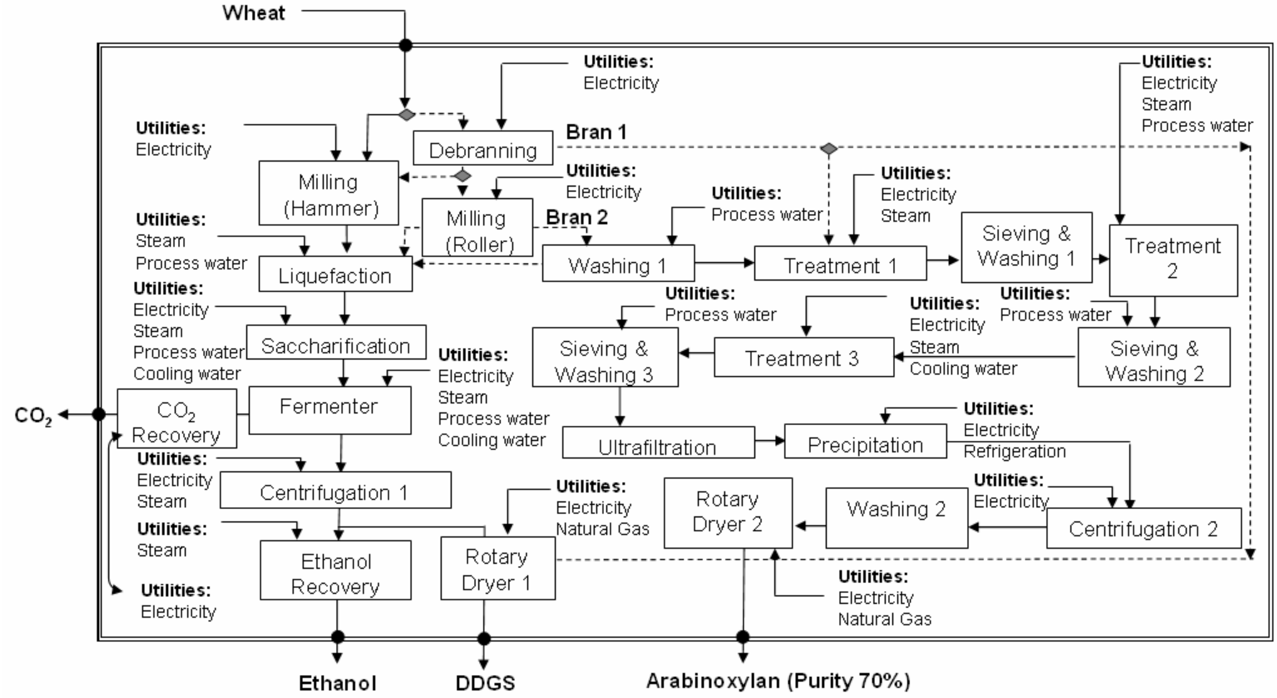


Figure 2.10. Superstructure showing all utility requirements for the proposed flowsheets.

2.5. Process integration

Integration and assessment tools are used already for other industrial systems, having been developed over many years (Smith, 2005). A general methodology, the Value Analysis Method, has been applied to wheat-based biorefineries in the current work. The approach systematically assesses various products and production routes in terms of Value on Processing (VOP) and Cost of Production (COP). The difference between these values provides the economic contribution of each individual stream.

2.5.1 Value Analysis Method

The Value Analysis Method (Sadhukhan *et al.*, 2003, 2004; Sadhukhan and Smith, 2006) has been developed and exploited in the areas of process network retrofitting and flowsheet selection. A key benefit of applying the method is that it provides transparency in analysing and optimising a process network. The stage-wise design analysis breaks the bigger problem into smaller solvable sub-problems, where the available integration opportunities at each level are captured, without sacrificing the solution quality.

The Value Analysis calculations are demonstrated through a simple example shown in Figure 2.11. The facility has a key input (wheat) and three key output products: Ethanol, DDGS, and CO_2. The various other streams are numbered 1-6. Every stream is characterised by a Value on Processing (VOP) and a Cost of Production (COP) where

- **COP** = Cost of the feedstock plus the operating costs of the upstream units that have contributed to the production of the stream
- **VOP** = Market value of its end product subtracted by the operating costs of the downstream units processing the stream

The COP values for wheat and the VOP values for products are equal to their market values. Other values are computed as shown in Table 2.1. The economic margin of each stream is equal to VOP–COP. Furthermore, the economic margin for wheat (VOP(wheat) – COP(wheat)) is equal to the overall economic margin of the facility.

Once the complete economic value structure of a process network is deduced, the weakest links and the missed opportunities in the network infrastructure can be identified. Non-profitable products could be constrained to the minimum production levels possible. Optimisation of a process network is also possible through market integration, overall integration among various processing elements, and improvement of the non-profitable/less profitable process (Sadhukhan *et al.*, 2004). Table 2.2 illustrates some of the key insights provided once all the COP/VOP values are computed.

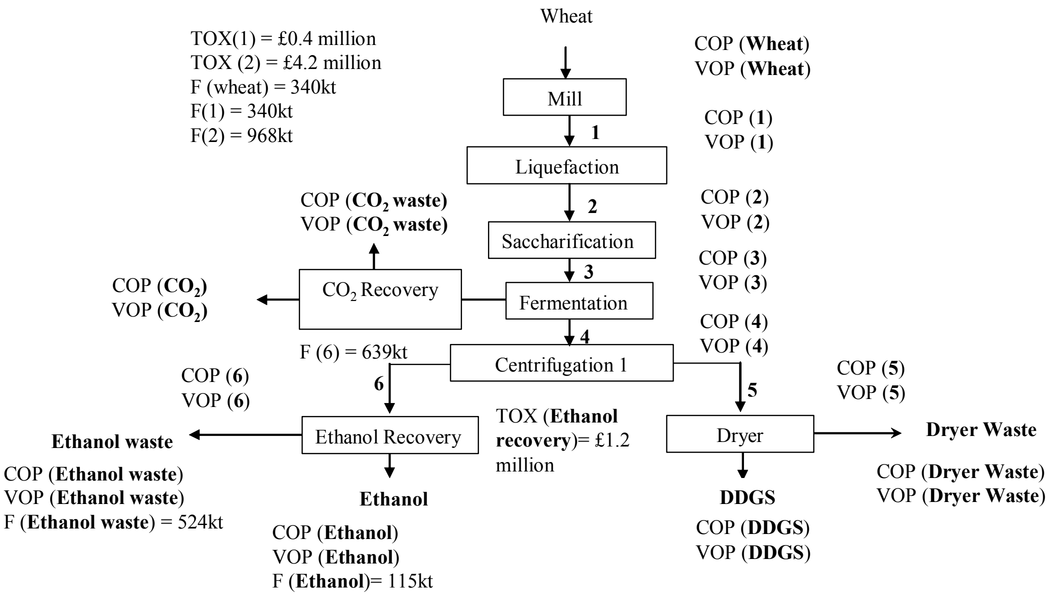


Figure 2.11. Value Analysis Method (Conventional bioethanol production).

Table 2.1. An example of COP/VOP calculations. TOX(*X*) is the total operating cost of operation to produce stream *X*, F(*X*) is the throughput to the operation.

Stream	COP calculations
Wheat	Market value = £96/t
1	$=\frac{(\text{COP(wheat)}\times\text{F(wheat)}+\text{TOX(1)})}{\text{F(1)}}$ $=\frac{((£96/\text{t}\times 340{,}000\text{t})+(£0.4\ \text{million}))}{(340{,}000\,\text{t})}=£97.18/\text{t}$
2	$=\frac{(\text{COP(1)}\times\text{F(1)}+\text{TOX(1)})}{\text{F(2)}}$ $=\frac{((£97.18/\text{t}\times 340{,}000\text{t})+(£4.2\ \text{million}))}{(968{,}000\ \text{t})}=£38.47/\text{t}$
Other streams	The same procedure is repeated for other streams until all the COP values downstream are computed. Note that if a unit has more than one stream, the COP values are assumed to be the same.

Stream	VOP calculations
Ethanol	Market value = £590/t
Ethanol Waste	Assume equal to £0/t
6	$=\frac{(\text{VOP(E)}\times\text{F(E)}+(\text{VOP(EW)}\times\text{F(EW)})-\text{TOX(ER)})}{\text{F(6)}}$ $=\frac{(£590/\text{t}\times 115{,}000\text{t})+(£0/\text{t}\times 524{,}000\text{t})-(£1.28\ \text{million})}{(639{,}000\,\text{t})}$ = £104.19/t (E refers to ethanol, EW to ethanol waste, and ER ethanol recovery)
Other streams	The same procedure is repeated until all the VOP values upstream are computed.

Table 2.2. Key insights provided by the Value Analysis Method.

Result	Key insight
VOP>COP	Profitable stream
COP>VOP	Nonprofitable stream
VOP (wheat) –COP (wheat)	Overall economic margin for complete facility
Lowest economic margin (min(VOP–COP))	Weakest stream

2.5.2 Ethanol integration

Figure 2.12 shows the integrated ethanol flows for bioethanol production and the AX extraction facility. 96% ethanol, from the ethanol recovery stage, is fed into the Precipitation and the Washing 2 steps. The ethanol is then recovered from the waste stream from Centrifugation 2 and Washing 2. This combined stream is then mixed with ethanol from the ethanol recovery stage to meet the requirements for Treatment 1 and Sieving and Washing 1. The waste streams from those two units are then sent back to the ethanol recovery stage.

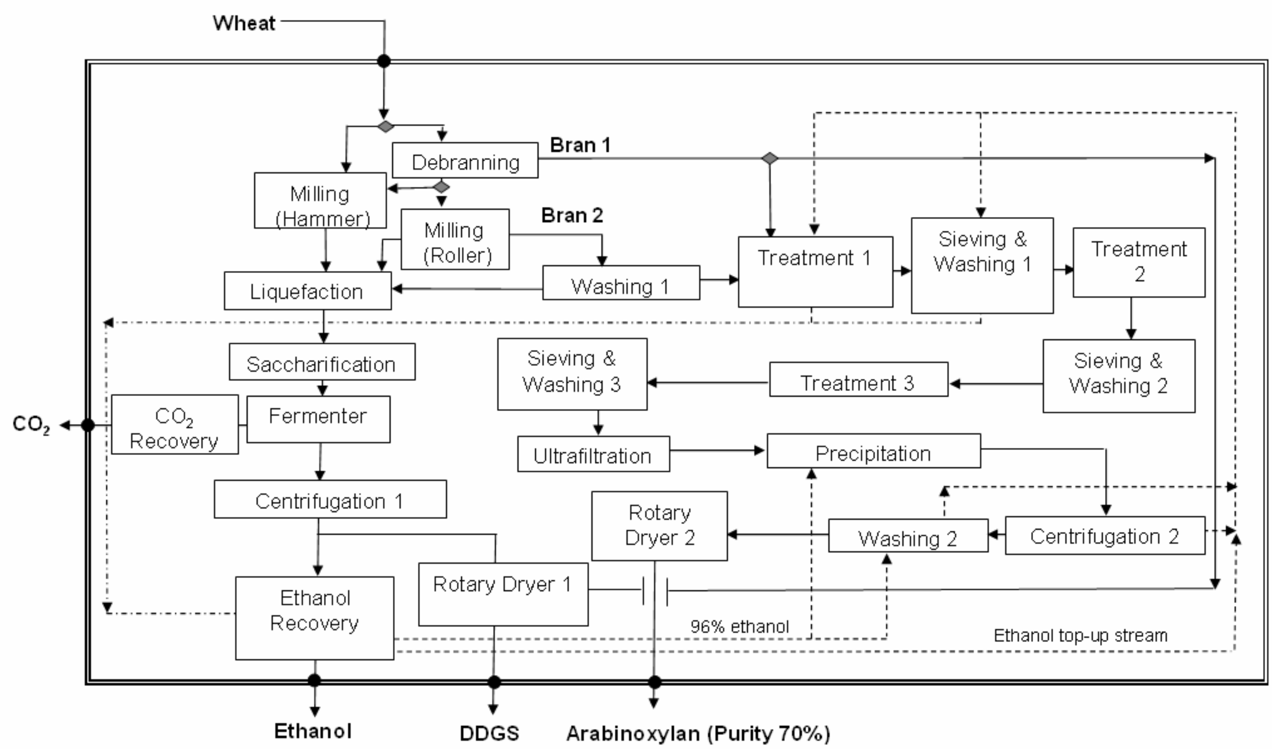


Figure 2.12. Ethanol integration with AX extraction.

2.6 Implementation as a software package

Various software tools are available (HYSYS, Aspen, Pro/II) which are able to simulate steady and dynamic states of different flowsheets. However, there is no current specialised software tool which provides a holistic and integrated capability to asses the economic potential of different biorefinery flowsheet options.

The software tool has been implemented using Microsoft Excel® (Microsoft Corporation, Redmond, WA). The main reason for its selection is the ability to transfer the model to various users without the prior requirement of installing expensive software tools and developing the necessary expertise in their use. A detailed description of the developed tool is provided in Appendix A.

2.6.1 Data gathering

The developed Excel models were populated with data acquired from various sources including literature (Sinnott, 2003; Anonymous, 2004; Hollmann and Lindhauer, 2005; Kwiatkowski *et al.*, 2006), industrial partners (Green Spirit Fuels and Satake), Aspen HYSYS simulations, and experimental studies. More detail into the range of data collected is provided in the following subsections. A full list of all data inputs and their sources is shown in Appendix B.

2.6.2 Literature

The work done by Kwiatkowski *et al.* (2006) provided the bulk of the data required for the simulation of the standard ethanol production method. Kwiatkowski *et al.* (2006) developed models, using SuperPro Designer software, to fully capture a conventional corn dry-grind processing facility producing 119 million kg/year of ethanol. Although their work is based on corn, much of the operational data is assumed to be similar for a wheat-based facility. Data on utility costs are based on Sinnott (2003).

2.6.3 Aspen HYSYS

Whenever utility requirements were not available from the literature, steady-state simulations were performed using the Aspen HYSYS simulation package (Aspen Technologies Inc., Cambridge, MA). Simulations include computing utility requirements for the following:

CO_2 recovery

Two units were simulated: a compressor and a cooler. The compressor increases the CO_2 pressure to 24 bar and the resulting liquid stream is then cooled to –30°C.

Treatment 1-4 (Arabinoxylan extraction)

The duties required to heat and cool the various streams were calculated. The liquids assumed were water or ethanol-water mixtures and the impact of solids was not included. Furthermore, the duty required to maintain the temperatures for certain durations, following heat losses, was not included.

Precipitation

The duty required to cool the stream coming from the ultrafiltration unit to 4°C was calculated.

Arabinoxylan drying

The duty required to heat the AX stream to 80°C (just over the boiling point for ethanol) was computed without the inclusion of AX. This was due to the unavailability of AX within the components available in the package.

2.6.4 Industrial Collaboration

Data obtained from the Home-Grown Cereals Authority, Green Spirit Fuels and Satake was crucial for the economic analysis. A full list of all the data gathered can be found in Appendix B.

2.6.5 Experimental studies

Experimental studies were conducted in the Satake Centre for Grain Process Engineering to measure the composition of a representative wheat bran and to determine the percentage recovery of starch, protein and arabinoxylan following a bran washing step prior to extraction. The results suggested that for this particular wheat, the arabinoxylan was concentrated in the outer layers. They also indicated that bran washing with water results in 70-75% recovery of starch. The complete experimental results are presented in Chapter 4.

2.7 Description of the Excel-based software tool

The tool is divided into three main sections. First, an input section allows the user to enter information regarding raw material, utilities and equipment. A second section contains the main engine behind the tool and focuses on the computation of mass balances and the operating costs. The final section involves the output of both mass balance and Value Analysis results.

2.7.1 User input

The following sections can be modified by the user:

- Assumptions
- Equipment detail
- Raw material input
- Utility input

2.7.1.1 Assumptions

This section allows the user to specify the following

- Facility operation
- Annual wheat intake
- Annual operating days
- Wheat/Bran composition
- Raw material and utility costs

2.7.1.2 Equipment detail

This section allows the user to specify the step yield of the various unit operations.

2.7.1.3 Raw material input

This section allows the user to specify the raw material requirements for the various unit operations.

2.7.1.4 Utility input

This section allows the user to specify the utility requirements for the various unit operations.

2.7.2 Calculations

2.7.2.1 Raw material costs

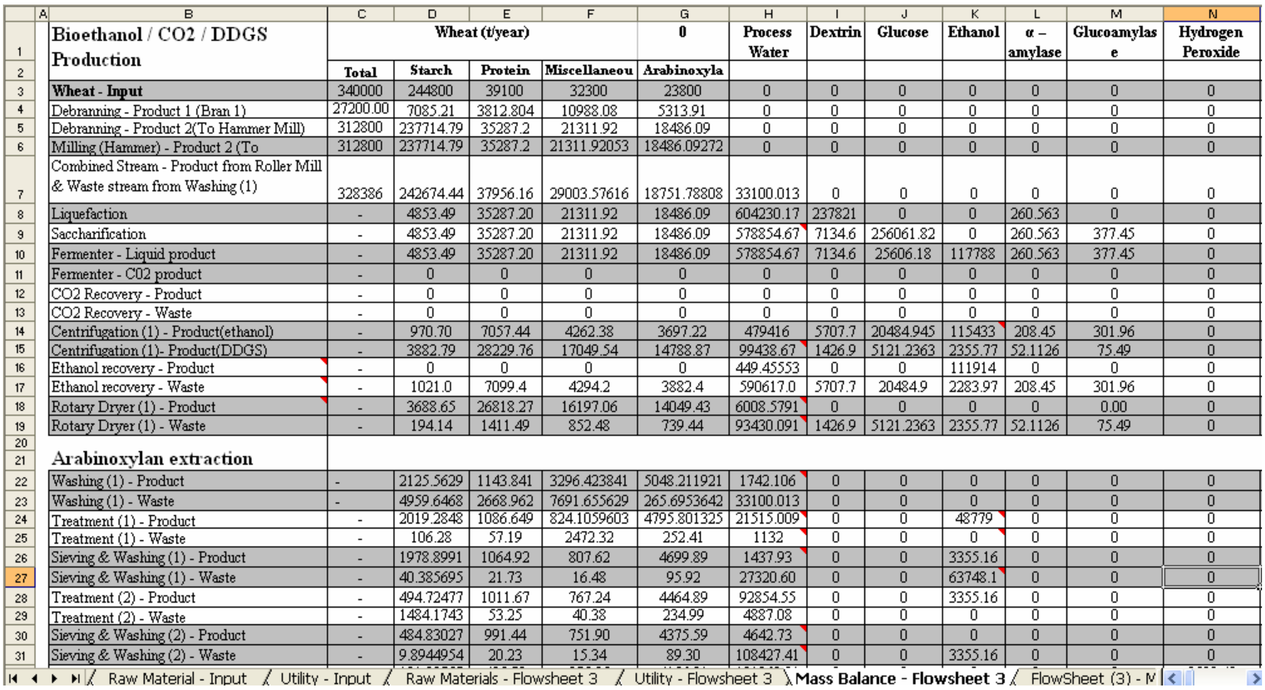
This section calculates the costs of the raw materials consumed in the various unit operations.

2.7.2.2 Utility costs

This section calculates the costs of the utilities consumed in the various unit operations.

2.7.2.3 Mass balance

This section contains the main calculation for the software tool which encompasses the mass balance calculations for the complete facility as well as the ethanol integration. Other recycles are not considered due to the very limited information available. The models included yield-based relationships between inputs and outputs. A number of built-in modelling assumptions are included as listed in Appendix B. Figure 2.13 shows part of the developed tool in Excel where the mass balance calculations are performed for a biorefinery producing ethanol, DDGS, CO_2 and AX, the latter at 80% purity. Raw materials are shown in the various columns, while input/output streams are shown on the various rows. The top section of the mass balance calculates the value of streams for the starch-exploiting section of the process where ethanol, DDGS, and CO2 are produced. The lower part then focuses on the bran-exploiting section where AX is produced. Due to space restrictions only part of the entirety of raw materials and process streams is shown.



	B	C	D	E	F	G	H	I	J	K	L	M	N
1	**Bioethanol / CO2 / DDGS Production**	**Wheat (t/year)**				**0**	**Process Water**	**Dextrin**	**Glucose**	**Ethanol**	**α – amylase**	**Glucoamylase**	**Hydrogen Peroxide**
2		**Total**	**Starch**	**Protein**	**Miscellaneou**	**Arabinoxyla**							
3	**Wheat - Input**	340000	244800	39100	32300	23800	0	0	0	0	0	0	0
4	Debranning - Product 1 (Bran 1)	27200.00	7085.21	3812.804	10988.08	5313.91	0	0	0	0	0	0	0
5	Debranning - Product 2(To Hammer Mill)	312800	237714.79	35287.2	21311.92	18486.09	0	0	0	0	0	0	0
6	Milling (Hammer) - Product 2 (To	312800	237714.79	35287.2	21311.92053	18486.09272	0	0	0	0	0	0	0
7	Combined Stream - Product from Roller Mill & Waste stream from Washing (1)	328386	242674.44	37956.16	29003.57616	18751.78808	33100.013	0	0	0	0	0	0
8	Liquefaction	-	4853.49	35287.20	21311.92	18486.09	604230.17	237821	0	0	260.563	0	0
9	Saccharification	-	4853.49	35287.20	21311.92	18486.09	578854.67	7134.6	256061.82	0	260.563	377.45	0
10	Fermenter - Liquid product	-	4853.49	35287.20	21311.92	18486.09	578854.67	7134.6	25606.18	117788	260.563	377.45	0
11	Fermenter - C02 product	-	0	0	0	0	0	0	0	0	0	0	0
12	CO2 Recovery - Product	-	0	0	0	0	0	0	0	0	0	0	0
13	CO2 Recovery - Waste	-	0	0	0	0	0	0	0	0	0	0	0
14	Centrifugation (1) - Product(ethanol)	-	970.70	7057.44	4262.38	3697.22	479416	5707.7	20484.945	115433	208.45	301.96	0
15	Centrifugation (1)- Product(DDGS)	-	3882.79	28229.76	17049.54	14788.87	99438.67	1426.9	5121.2363	2355.77	52.1126	75.49	0
16	Ethanol recovery - Product	-	0	0	0	0	449.45553	0	0	111914	0	0	0
17	Ethanol recovery - Waste	-	1021.0	7099.4	4294.2	3882.4	590617.0	5707.7	20484.9	2283.97	208.45	301.96	0
18	Rotary Dryer (1) - Product	-	3688.65	26818.27	16197.06	14049.43	6008.5791	0	0	0	0	0.00	0
19	Rotary Dryer (1) - Waste	-	194.14	1411.49	852.48	739.44	93430.091	1426.9	5121.2363	2355.77	52.1126	75.49	0
20													
21	**Arabinoxylan extraction**												
22	Washing (1) - Product	-	2125.5629	1143.841	3296.423841	5048.211921	1742.106	0	0	0	0	0	0
23	Washing (1) - Waste	-	4959.6468	2668.962	7691.655629	265.6953642	33100.013	0	0	0	0	0	0
24	Treatment (1) - Product	-	2019.2848	1086.649	824.1059603	4795.801325	21515.009	0	0	48779	0	0	0
25	Treatment (1) - Waste	-	106.28	57.19	2472.32	252.41	1132	0	0	0	0	0	0
26	Sieving & Washing (1) - Product	-	1978.8991	1064.92	807.62	4699.89	1437.93	0	0	3355.16	0	0	0
27	Sieving & Washing (1) - Waste	-	40.385695	21.73	16.48	95.92	27320.60	0	0	63748.1	0	0	0
28	Treatment (2) - Product	-	494.72477	1011.67	767.24	4464.89	92854.55	0	0	3355.16	0	0	0
29	Treatment (2) - Waste	-	1484.1743	53.25	40.38	234.99	4887.08	0	0	0	0	0	0
30	Sieving & Washing (2) - Product	-	484.83027	991.44	751.90	4375.59	4642.73	0	0	0	0	0	0
31	Sieving & Washing (2) - Waste	-	9.8944954	20.23	15.34	89.30	108427.41	0	0	3355.16	0	0	0

Figure 2.13. A snapshot of the mass balance section of the tool.

2.7.3 Outputs

2.7.3.1 Results – Mass balance

This section contains a flowsheet with the mass balance outputs presented for each individual stream.

2.7.3.2 Results - Value analysis

This section contains a flowsheet with the value analysis outputs presented. For each stream the Cost of Production, Value on Processing and the economic margin are presented.

2.7.4 Model verification and validation

The results were validated using SuperPro Designer, a commercial software package. The two software tools gave comparable results.

One of the very important features of any robust software tool is the ability to deal with errors. Thus an error handling facility for dealing with negative values in the mass balance calculations, due to wrong user inputs, has been added. In the case of a negative value occurring in the mass balance, the software tool section within the start worksheet will show the message “Mass balance error”. So it is important to check the message after each simulation and to make sure that it is showing “Successful”. The main cause of this error is when the user specifies a composition for wheat or bran that is not compatible with the specified percentage of bran extracted.

2.8 Adapting the methodology to other scenarios

The developed approach could be adapted to other scenarios such as Succinic acid production. The key challenges lie in data and knowledge acquisition. Experimental data are likely to be required. Process simulators such as Aspen HYSYS provide a useful tool for computing utility requirements.

One of the key benefits of the value analysis method is that it provides transparency in analysing and optimising flowsheets. The methodology allows the identification of the weakest streams, thereby highlighting areas for improvement. It also allows the computation of the economic contribution from each stream and hence speeds up the process of flowsheet selection. The approach has shown that the raw material and utility costs, which make up the bulk of the operating cost, are acceptable at the conceptual design stage.

Concerning process integration, CO_2 integration would be possible within a biorefinery producing succinic acid and bioethanol, since ethanol production produces CO_2, while succinic acid production consumes CO_2.

2.9 Summary

This chapter describes conventional ethanol production and the most appropriate available process for AX extraction within an integrated biorefinery. The choice of extraction method, using ethanol precipitation, allows the direct integration with ethanol production. Four flowsheets were initially proposed, in collaboration with industrial partners, to present different ways of exploiting the bran fraction. A process integration approach, the Value Analysis Method, was adopted. The software tool was implemented using Excel and thus does not require prior installation of expensive software packages. The data gathered was from a number of sources including literature, Aspen HYSYS process simulations, industrial collaboration, and experimental studies. The next chapter presents the analysis based on this tool and the preliminary design conclusions drawn.

3. Conceptual design

3.1 Introduction

This chapter presents an initial study, based on the developed value analysis framework for biorefineries in Excel, for flowsheet selection. The operating costs are assumed to include raw material and utilities only. Additional costs (*i.e.* capital investment and labour costs) are not considered at this stage, but are included later in Chapter 5, within the rigorous simulations performed using SuperPro Designer.

The first section provides the analysis for the base case assuming a conventional bioethanol production route. Then, a comprehensive debranning analysis is provided to address the issue of whether debranning, for its own sake, provides any economic benefit. Finally, the basis for flowsheet selection is presented.

3.2 Conventional bioethanol production

Using the Excel-based model described in the previous chapter, the overall economic margin is calculated as £96.67 per tonne of wheat processed on the basis of a wheat-based biorefinery processing 340,000 t of wheat per annum. However, the economic margin is not purely profit since other costs, such as capital investment and labour cost, are not included. The total operating cost of the facility is £40.9 million which corresponds to £120.19 per tonne of wheat processed. The results show that 90% of the total operating cost is made up of raw materials whereas the utilities count for only 10%. Furthermore, Table 3.1 shows how the raw material fraction is mainly due to the contribution of the cost of wheat (~89%). Concerning the utilities, the highest costs are due to consumption of steam, electricity and natural gas (Table 3.2). This is also reflected in Table 3.3 with the highest costs of operation due to the ethanol recovery and liquefaction stages, where there is a high consumption of steam.

Table 3.1. Total raw material costs breakdown.

Raw material	% of total raw material cost
Wheat	88.8
Sodium Hydroxide	7.4
Enzymes	3.6
Miscellaneous	0.2

Table 3.2. Total cost of utility breakdown in terms of utility consumption.

Utility	% of total utility cost
Steam	41.4
Electricity	28.3
Natural gas	18.1
Process water	9.1
Cooling water	3.1

Table 3.3. Total cost of utility breakdown in terms of operation.

Operation	**% of total utility cost**
Ethanol recovery	31.3
Liquefaction	22.0
Rotary Dryer	20.4
CO_2 recovery	11.3
Hammer milling	10.0
Centrifugation	2.4
Fermenter	2.2
Saccharification	0.5

Figure 3.1 shows how the overall economic margin for the facility is most sensitive to changes in the price of ethanol and wheat, and least sensitive to process water and cooling water prices. Batchelor *et al*. (1994) similarly found bioethanol production to be highly sensitive to wheat price and moderately sensitive to DDGS price.

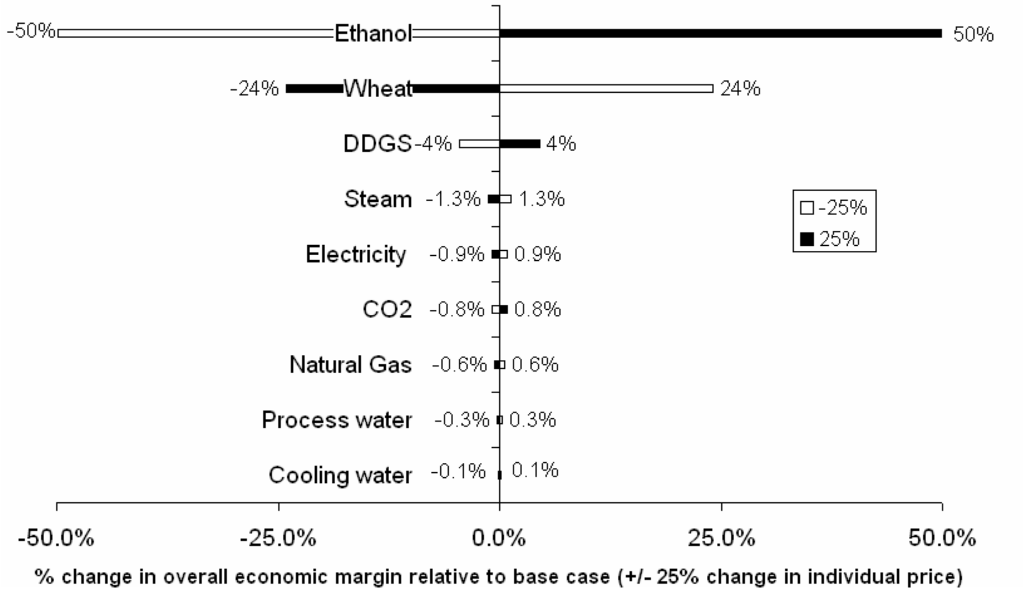


Figure 3.1. Impact of a ±25% change in individual price of various raw materials, products, and utilities, on the overall economic margin. The total economic margin improves with an increase in the price of products (ethanol, DDGS, and CO_2), whereas it deteriorates with an increase in the price of raw materials and utilities.

3.3 Economic assessment of removing bran for direct addition to DDGS

The bran particles are suspended in the mash during the several processing steps of a conventional dry milling bioethanol route and are finally present in the DDGS product stream. The non-starch polysaccharides that are concentrated in the bran particles have the ability to absorb a large amount of water. This fact renders the mash even more viscous, which increases the electricity requirements for agitation and solids handling for the DDGS processing and also increases the process water requirements, giving higher steam requirements for the DDGS drying, and increasing of the size of the processing tanks for liquefaction, saccharification and fermentation. It is therefore worthwhile to consider the option of removing some of the bran via debranning and sending this directly to DDGS, thereby avoiding the addition of water to this bran and the consequent increases in drying and electricity costs. However, this must be offset against the fact that the debranning procedure itself is a significant electricity consuming operation. In addition, there is the additional capital cost of the debranner. Ignoring this for the moment, the first question is whether the savings in drying and electricity costs by removing some of the bran and bypassing the ethanol process are greater than the cost of the electricity consumed by the debranner.

Flowsheet 2 (Figure 2.5) describes the process. The trade off between the conventional route (Flowsheet 12, Figure 2.4) and the debranning alternative was examined by developing an Excel spreadsheet using data from Kwiatkowski *et al.* (2006). In this spreadsheet the debranning system removes the outer layers of the wheat up to 10% w/w of the initial grain. The greater the degree of debranning, the less process water is required for the bioethanol production (resulting in less steam consumption to dry the DDGS and less electricity for agitation of the tanks). The following assumptions were made:

- The parameters that affect the comparison are mainly the steam consumption, the electricity consumption and the depreciation of the several processing tanks.
- The electricity consumption of the debranning procedure is always constant through the several debranning percentages. The additional electricity requirement of the debranner is always 650 kW, irrespective of the degree of debranning achieved. This is the power rating of a debranner suitable for a wheat processing facility of this scale (A Bailey, personal communication, 2006).
- The depreciation takes into consideration only the necessary tanks of the bioethanol processing. It does not consider the cost of the debranner, the evaporator, the centrifuge and other basic equipment, for which accurate cost estimation is difficult.

The major disadvantage of the debranning alternative is that considerable quantities of starch are lost to the bran-rich stream. Table 4.1 in the next chapter shows the starch contents of bran removed to several different degrees. The greater the degree of debranning, the more starch the bran-rich stream contains. If the bran is sent directly to the DDGS stream, ethanol yield will be considerably reduced. For the simulation, the ethanol losses were accounted for in the debranning alternative assuming an ethanol price of 0.35 £/kg.

Figure 3.2 identifies the utility requirements of the conventional route and the 10% w/w removal alternative of the several major sections of the bioethanol production. Ignoring the additional electricity consumption of the debranner itself, electricity usage in the rest of the process is reduced, along with steam and process water. Figure 3.3 shows the total considered costs in respect of the debranning percentage expressed on a per kg of wheat processed basis, considering also the starch losses. The upward trend of the total costs reflects the fact that the extra cost associated with starch losses exceeds the reduction in costs of electricity and steam. The contribution of those costs in the conventional process is about 0.012 £/kg of wheat processed. The decrease in depreciation arising from the use of smaller equipment when employing debranning is only slight, showing that this factor does not affect the economics as much as starch losses. An additional washing step with water in order to recover 70-75% of the starch would be feasible, but it would render the particles wet. The drying of these particles would increase the steam costs to levels similar to those of the conventional route, thus eliminating the advantage of the debranning alternative. The debranning alternative for the removal of part of the bran directly to the DDGS stream is therefore more expensive than the conventional route, mainly because of the starch losses. Even ignoring these, the additional electricity consumption of the debranner exceeds the various other cost savings. On top of this, considering the capital cost of the debranner reinforces the conclusion that this approach would not be economical.

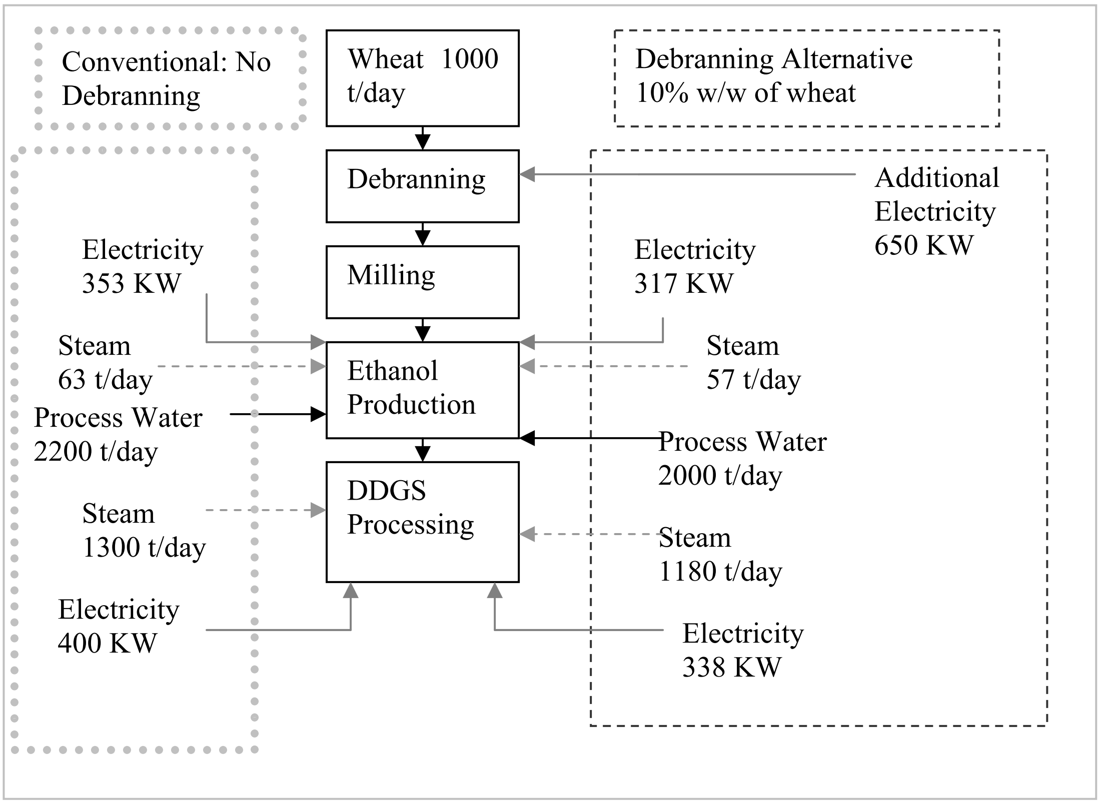


Figure 3.2. The utility requirements of ethanol production with and without debranning.

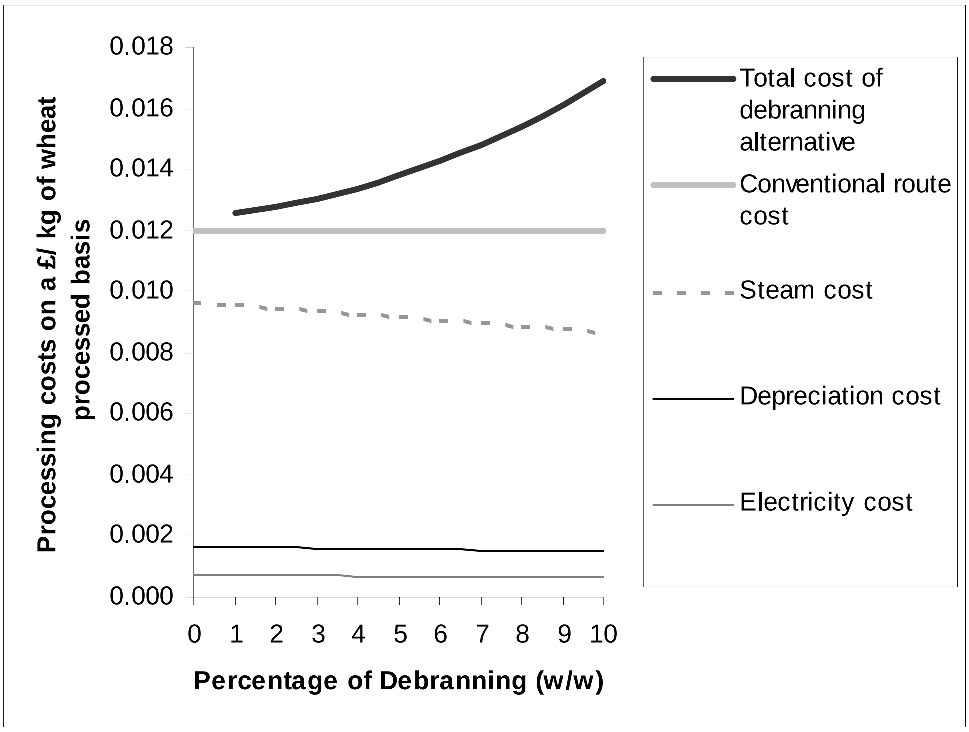


Figure 3.3. Comparison of the considered costs at different debranning percentages.

A sensitivity analysis was also conducted using the composition for 8% bran (Table 4.1). The starch composition was varied by ±25% to see the impact on the overall economic margin. The results showed again that the overall economic margin is mainly sensitive to starch losses in bran, which translates into ethanol losses. An overall economic margin of –3.1% and –0.65% was achieved (relative to the ethanol production base case) with a +25% and –25% change in starch composition in the removed bran, respectively. Variations in other bran components had a negligible impact on overall economics.

The conclusion is that employing debranning to remove bran and sending it directly to DDGS (in order to reduce the amount of bran passing through the fermentation process) is not beneficial. Debranning is therefore only worth employing if the bran is then sent for further processing such as AX extraction. Even then, this is only worthwhile if the bran obtained in this way contains substantial amounts of functional AX, and if debranning gives economic advantages over other methods of obtaining bran. These issues are addressed in Chapters 4 and 5.

3.4 Flowsheet selection

Various types of bran could be used for arabinoxylan extraction. Bran could be collected using a debranner, a roller mill, or even after hammer milling using a sieve. The latter is the cheapest but the least efficient option.

At this stage, certain specifications are clearly emerging at the conceptual level for the best flowsheet:

- It should not involve sending bran to DDGS. This clearly would present no economic benefit, and hence both Flowsheet 2 (debranning and sending bran to DDGS) and Flowsheet 3 (partly sending bran to DDGS and partly to AX extraction) options could be eliminated.
- It should fully integrate bioethanol within the biorefinery.
- It should recover any starch remaining in the bran and send it back to the liquefaction stage.
- Furthermore, it can be safely assumed that it is much better to recover AX using the debranning option instead of the roller milling option due to the following reasons: (a) Experimental results show that AX seems to be concentrated on the outer layers of wheat which could be extracted using a debranner; and (b) The utility consumption (electricity) for debranning is less than for roller milling (for which several milling and sifting stages would be required to give a reasonably clean bran).

Concerning starch recovery from bran, experimental results presented in the next chapter showed that 70-75% recovery of starch is possible through the introduction of a bran washing step. A similar value is assumed for the recovery of other bran components (such as protein), while a 5% loss of AX is assumed. Based on the experimental values and the assumptions for bran component recovery, the impact of the change in price of AX on the economic margin is presented in Figure 3.4. The results show that the minimum market value for AX at 70% purity is around £1500/t and around £2355/t for an 80% purity product. The results are based on the facility's ability to break even, in terms of achieving a similar overall economic margin when compared with the conventional bioethanol base case. However, these market values for AX do not consider at this stage other costs such as capital investment and labour. This analysis therefore reflects the plausible scenario in which an AX extraction facility is available, with the decision being whether or not (under given raw material and marketing conditions) it should be operated. In this scenario it is not the capital investment that is the issue but just the operating costs versus the extra revenue. Simulation of the alternative (and more realistic) scenario of deciding whether to invest in AX extraction based on full consideration of capital and operating costs is presented in Chapter 5.

A closer look at the production of a higher purity (80%) product shows that the total annual operating cost is £45.4 million, which corresponds to £133.43 per tonne of wheat processed. This represents an increase of 11% in the total operating cost relative to the base case. Both flowsheets are compared on the basis of producing a similar economic margin. However, capital equipment and labour costs are not included. Figure 3.5 shows the sensitivity of the overall economic margin to ethanol and AX price. It is clear that the economics are much more sensitive to ethanol price than to the price of AX, as the contribution of the former to the total revenue is much higher.

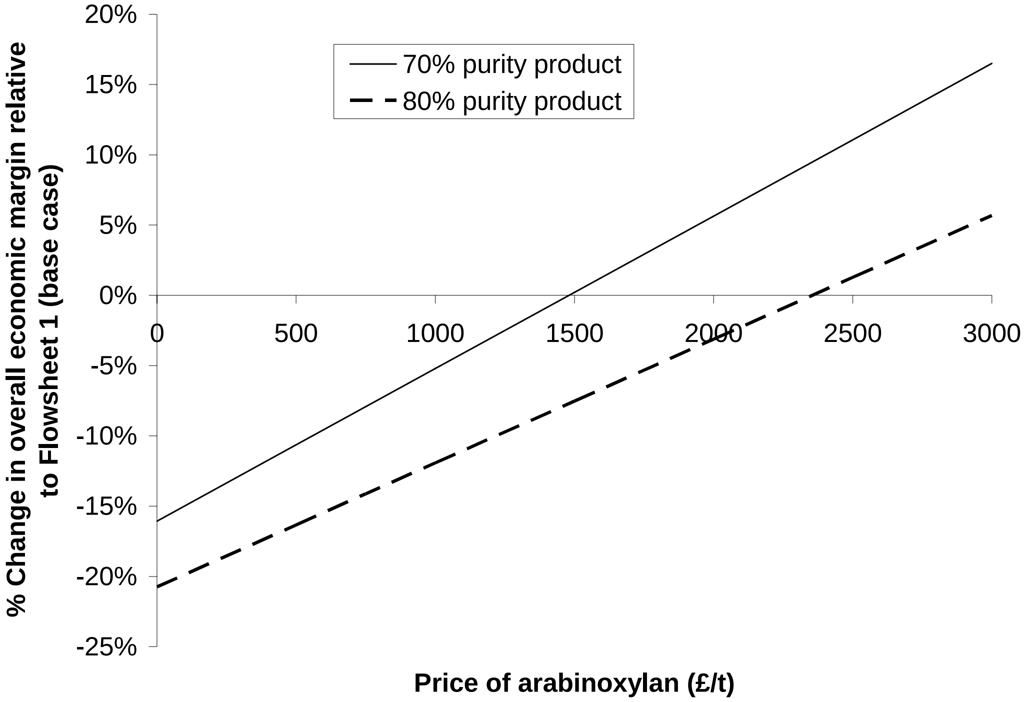


Figure 3.4. The impact of the change in price of AX on the overall economic margin, for 70% and 80% purity products.

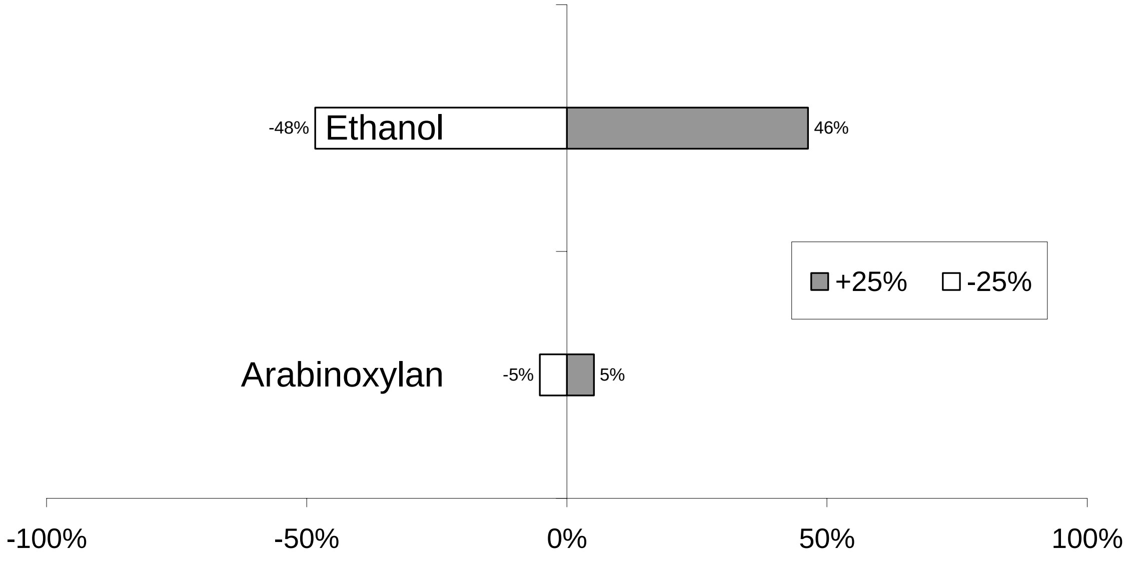


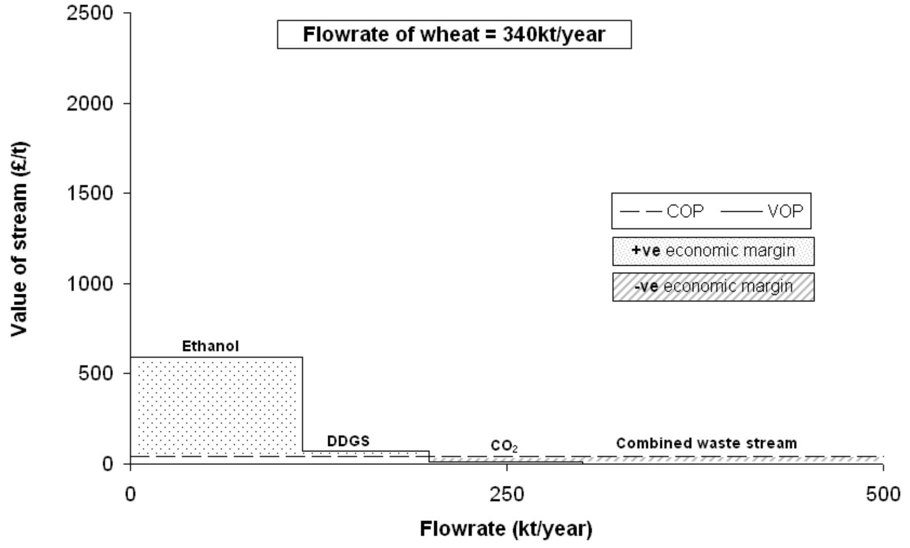
Figure 3.5. Sensitivity analysis of the overall economic margin, with change in ethanol and AX price, relative to base case (conventional bioethanol production).

Figure 3.6 shows the total economic margin breakdown for the bioethanol production base case and the further production of an 80% purity AX co-product. The *y*-axis shows the various COP/VOP values for the main streams whereas the flowrates are shown on the *x*-axis. All waste streams are presented as a combined waste stream which is mainly composed of water. The flowrate of the combined waste stream continues beyond 500 kt/year; however, only a small section is shown in order to focus on the value analysis results for the key streams. The area under the graph, defined by the flowrate of each stream times its economic contribution (VOP–COP), represents the economic margin of a stream in £. The resulting positive and negative economic margins are clearly highlighted.

Figure 3.6a shows how the major contribution to the total economic margin is due to ethanol; the economic margin of ethanol is approximately 26 times that of DDGS. On the other hand, a closer look at CO_2 shows that although the value of the stream (VOP) is £10.7/t, it still fails to cover the COP of the stream of £43.47, giving a loss of £32.77 per tonne of CO_2 recovered. However, although the stream is not profitable, the addition of a CO_2 recovery step reduces the loss in economic margin from £39.39/t (without CO_2 recovery) to £32.77 per tonne of CO_2 processed. Depending on the capital costs for CO_2 recovery, this may be desirable.

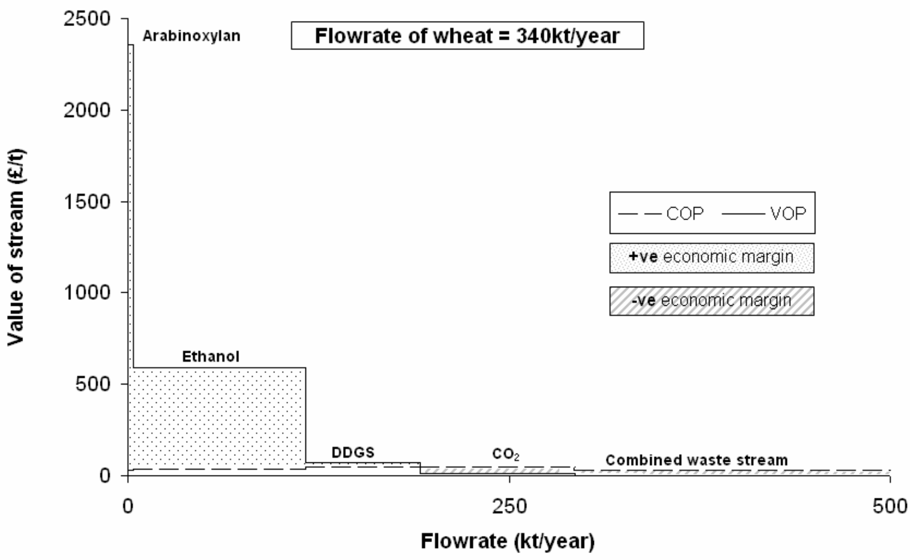
Figure 3.6b presents the market value of £2355/t of AX required to provide a total economic margin which is similar to the base case. This is due to the small flowrate of AX of 4,000 t per year. Selling AX at a price that exceeds its COP would result in a profitable stream; however, AX must have a much higher market value to cover the added costs incurred by the addition of the AX extraction process and by any losses in ethanol and/or DDGS production.

This is a preliminary analysis that excludes capital costs. As more economic and process data become available, the full potential of the Value Analysis Method could be realised. Optimisation of process networks could be achieved through (i) market integration, (ii) optimisation of network connections, and (iii) process optimisation. A simple example for market integration could be demonstrated through a scenario where VOP>COP>Market value for an intermediate stream. Considering the scenario for destarched bran fed into Treatment 1 for AX extraction, although the stream is profitable (VOP>COP), with a market value lower than both COP/VOP values, it is cheaper to buy the stream. Hence, a potential strategy could be to reduce production of bran and instead increase purchasing of destarched bran. This is valid assuming the functional properties of the extracted AX are not affected.



Stream	COP (£/t)	VOP(£/t)	Economic margin = VOP-COP (£/t)	Flowrate (kt)	Total (million £)
Ethanol	41.52	590	548.48	114.57	62.84
DDGS	43.39	72.5	29.11	83.6	2.43
CO2	43.47	10.7	-32.77	102.29	-3.35
Combined waste	41.93	0	-41.93	668.71	-28.04

a. Production of bioethanol, DDGS, and CO_2 (base case).



Stream	COP (£/t)	VOP(£/t)	Economic margin = VOP - COP (£/t)	Flowrate (kt)	Total (million £)
Arabinoxylan	27	2355	2328	4	8.56
Ethanol	37.98	590	552	113	62.15
DDGS	45.41	72.5	27.1	76	2.05
CO2	44.75	10.7	-34.1	101	- 3.45
Combined waste	28.61	0	-28.6	1238	- 35.42

b. Production of an additional 80% purity arabinoxylan co-product.

Figure 3.6. Detailed value analysis for a biorefinery (a) producing bioethanol, DDGS, and CO_2 (base case) and (b) co-producing an additional 80% purity AX product.

3.5 Summary

A number of proposed flowsheets that could boost the biorefinery economics were investigated. The initial analysis for the base case of conventional bioethanol production shows, not surprisingly, that operating costs are dominated by raw material costs and in particular by the cost of wheat. For the utilities, steam consumption contributes the highest cost. In terms of operations, the ethanol recovery stage has the highest utility costs.

Debranning and sending the removed bran directly to DDGS provides no economical benefit relative to the base case, due to the electricity consumption of the debranner itself, its capital cost, and starch losses with the bran that would reduce ethanol yield. Debranning is only worthwhile as a convenient means of obtaining bran for further processing, in this case for AX extraction. Experimental results from the next Chapter indicate that the bran obtained by pearling is enhanced in AX and gives higher yields on extraction. On this basis the use of a debranner is worthy of further consideration.

This preliminary flowsheet selection analysis based on the currently available data has shown that out of a number of options, the use of a debranner, incorporation of a washing step (to recover starch), and an AX extraction process show promise in terms of generating additional revenue for a biorefinery principally producing bioethanol. A cheaper alternative to using a debranner is simply to use a hammer mill, with sieving to recover larger bran particles and washing to recover some of the starch. These two options are therefore the ones selected for full analysis in Chapter 5. Figures 3.7 and 3.8 present these two flowsheets, for the production of an 80% purity AX product.

The analysis has not included costs such as capital investment and labour. In particular, consideration of the capital cost and other consequences of using a debranner may alter this preliminary conclusion and favour alternative ways of recovering bran for extraction. Chapter 5 presents a more comprehensive analysis using rigorous simulations in SuperPro Designer, and incorporating all capital and operating costs. Before this, however, the next Chapter presents some key information on AX concentrations and starch recovery based on experimental studies.

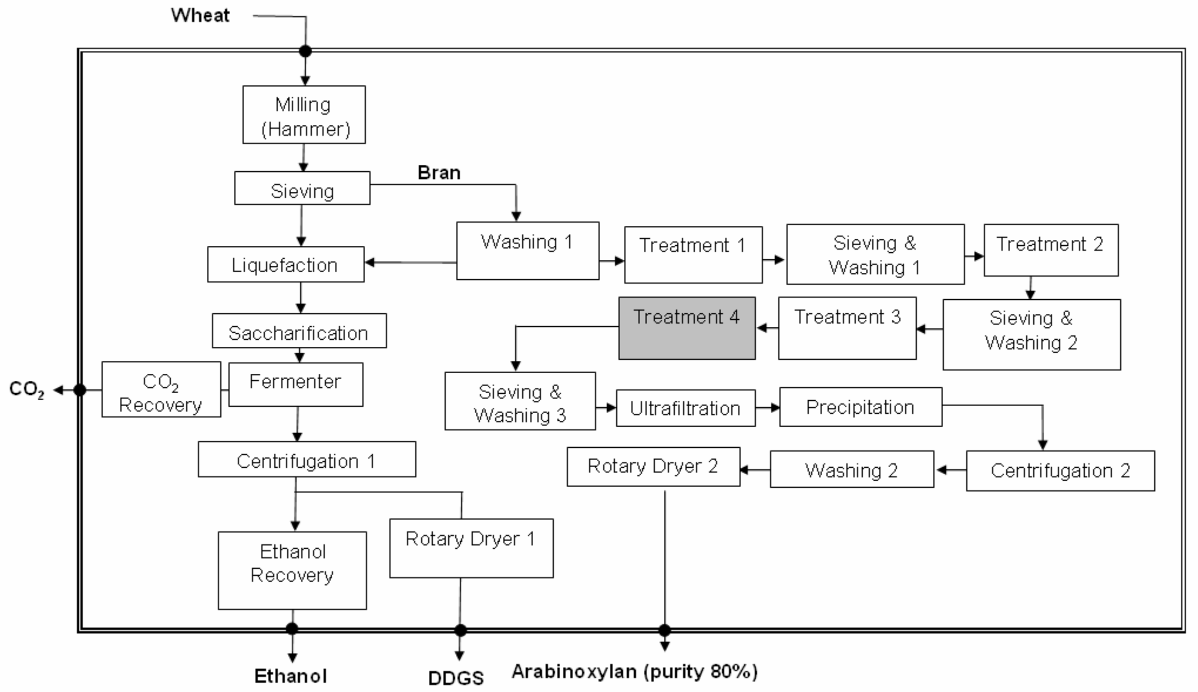


Figure 3.7. A proposed biorefinery producing ethanol, DDGS, CO_2 and an 80% purity arabinoxylan product using hammer milling and sieving to recover the bran.

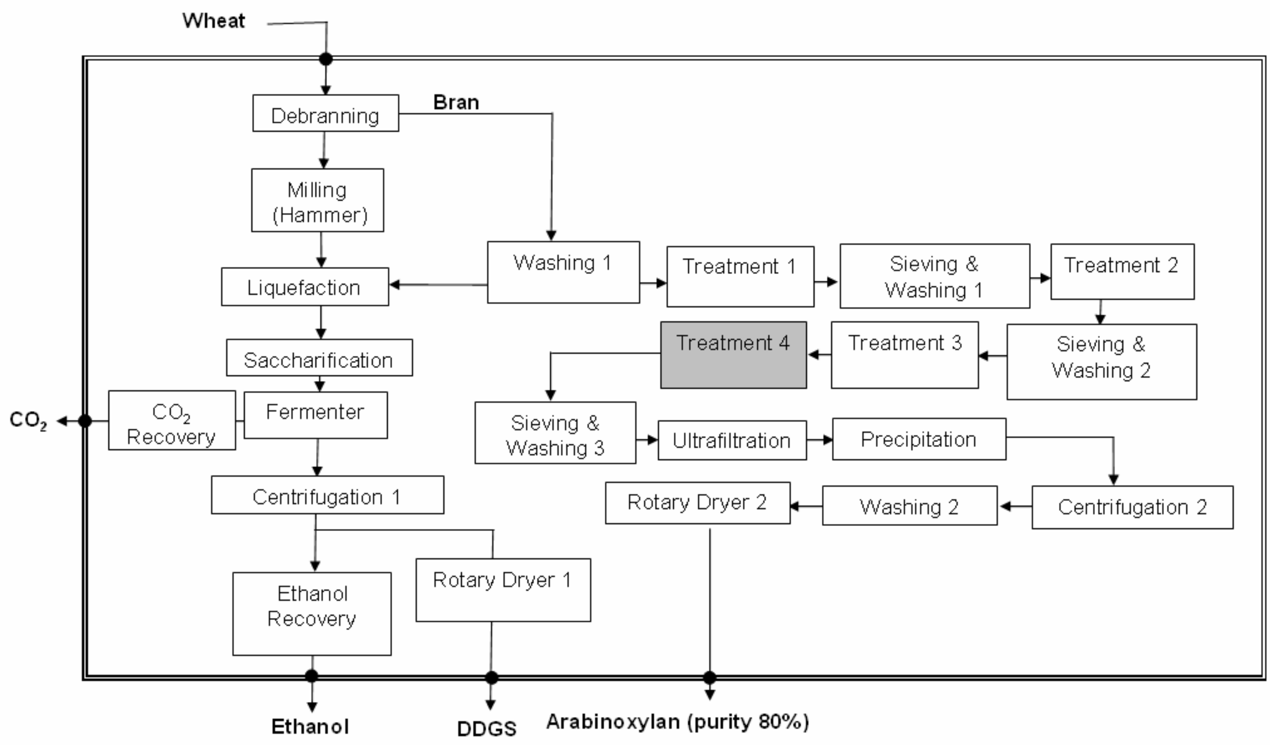


Figure 3.8. A proposed biorefinery producing ethanol, DDGS, CO_2 and an 80% purity arabinoxylan product using debranning to recover the bran.

4. Experimental studies of arabinoxylan extraction from wheat bran

4.1 Introduction

The flowsheets developed and analysed in the preceding section necessarily employed numerous assumptions regarding the composition of varying process streams and their ability to be processed. AX extraction from wheat bran in a plant-scale context has not been investigated previously, and there is no existing plant from which to obtain process data. Therefore, in order to support the simulations, experimental investigations of some of the key areas were undertaken. In particular, the question of whether bran recovered via pearling (debranning) contains an enhanced level of AX, or indeed any AX, was key. In addition, however bran is obtained, some starch is inevitably attached to the bran and if not recovered, would lead to yield losses of ethanol. Washing of the bran to recover this starch was therefore also investigated.

4.2 Materials and Methods

4.2.1 Production of bran samples for analysis and AX extraction

The wheat used in this study was Consort, a soft wheat variety harvested in 2003 and supplied by Wessex Grain Limited (Somerset, UK). A soft wheat variety was chosen for the study, as soft wheat (with lower protein and hence higher starch content) is most likely to be the feedstock for ethanol biorefineries. The wheat was pearled without conditioning in 180 g batches using the Satake TM05 laboratory debranner (Satake Corporation, Japan) to different levels of bran removal (4, 8 and 12% of the initial weight of the wheat). The partially pearled wheat kernels were then processed through the Bühler laboratory mills to produce flour and bran. Whole (unpearled) wheat was also Bühler milled to produce flour and bran. Thus a total of seven brans were produced, one from whole wheat, three from pearling to different degrees, and three from milling the pearled kernels. The composition of the seven bran samples, in particular their AX contents, were determined. The seven brans were then subjected to the AX extraction procedure.

4.2.2 Analytical methods

The contents of moisture, protein and ash in the wheat brans were measured using standard ICC methods (ICC, 1991). Starch content was analysed by an enzyme starch analysis kit (Megazyme Ltd., Ireland). Glucose concentration was determined by a glucose analyser (Analox, UK). To determine the AX content of wheat brans prior to extraction and of the extracted AX products, the procedure of Hollmann and Lindhauer (2005) was followed. Samples were firstly hydrolysed with sulphuric acid to liberate arabinose and xylose, which were then measured by High Performance Liquid Chromatography (HPLC, Star Varian Chromatography Workstation) with an evaporative light scattering detector (PL-ELS 2100, Polymer Laboratories). Samples of 10-20 mg were hydrolysed in 1 M sulphuric acid at 121°C for 1 h in an autoclave. The samples were neutralised with 0.25 M sodium hydroxide. The analytical column was a monodisperse, sulphonated styrene/divinylbenzene copolymer column (PL Hi-Plex H 8μm 300 × 7.7 mm, Polymer Laboratories) preceded by a guard column (PL Hi-Plex H Guard column 50 × 7.7 mm, Polymer Laboratories). The analysis was carried out under the following conditions: sample volume 20 μl, flow phase 0.1% (v/v) trifluoroacetic acid (TFA), flow rate 0.6 ml min^{-1}; column temperature 60°C (column oven: Jasco CO-965); neb = 50°C; evap = 80°C; gas = 1.6 SLM. Arabinose and xylose standards were of highest purity (98%) available and obtained from Fisher UK. The AX content of samples was calculated as 0.88×(Arabinose + Xylose). Glucuronic acid and galactose were not included in the calculations, thus the yields reported below are slightly underestimated compared with what would be calculated for commercial yields.

4.2.3 Isolation and purification of arabinoxylans

AX was extracted from the seven bran samples using a modified process based on the work of Hollmann and Lindhauer (2005). Wheat bran (50 g) was suspended in 300 ml ethanol (70% v/v) and incubated at 80°C in a water-bath for 4 h with stirring by a magnetic stirrer. After cooling to room temperature, the mixture was filtered and washed with 30 ml of 70% ethanol. The solid was dried in a 50°C oven for at least 12 h. To obtain water-extractable arabinoxylans (WEAX), the purified wheat bran was added to 400 ml of water which was then incubated in a 40°C water-bath for 2 h with constant stirring by a magnetic stirrer. Then the mixture was centrifuged at 4,000 rpm at room temperature for 15 min. The liquid was transferred into a 2 L Duran bottle. Industrial methylated spirit (IMS) was added to a final concentration of 65% (v/v) and the precipitated material was stored in a 4°C fridge overnight before filtration. The solid phase of the filtration was WEAX.

The alkali-extractable arabinoxylans (AEAX) exited in the solids following centrifugation. After drying for 24 h at a 50°C oven, the solids were suspended in 600 ml of 2% hydrogen peroxide and adjusted to pH 11 using 10 M sodium hydroxide solution, with 0.4 ml antifoam added into the mixture. The suspension was incubated in a 40°C water-bath for 4 h with stirring by a magnetic stirrer. After cooling to room temperature the pH of the mixture was adjusted to 8.5 with 98% sulphuric acid, and 1 ml Protease P4860 (Sigma) was added. After stirring for 12 h in a 20°C water-bath, the mixture was heated to 100°C for 10 min in a boiling water-bath. After cooling to room temperature, the pH was adjusted to 7 by 1 M sulphuric acid. Subsequently, the mixture was centrifuged at 4,000 rpm at room temperature for 15 min. The collected liquid was transferred into a 2 L Duran bottle. Industrial methylated spirit was added to a final concentration of 65% (v/v) and the precipitated material was put into a 4°C fridge overnight before filtration. The solids resulting from the filtration were collected and subjected to a β-glucan removal process by lichenase and β-glucosidase (Megazyme). The detailed procedures are described by Hollmann and Lindhauer (2005).

4.2.4 Investigation of the effectiveness of bran washing

Within the proposed industrial process, a bran washing stage is envisaged in order to recover starch from the bran and to return it to the fermentation section. In order to include the residual starch losses in the simulations, it was necessary to generate some representative data on the likely effectiveness of this bran washing step. The water washing experiment was carried out using a 1 L beaker. A 50 g sample of bran was suspended in 500 ml tap water and stirred by a magnetic stirrer for 30 min, with the temperature controlled at 30°C by a water-bath. Subsequently, bran particles were collected on a 0.212 mm sieve and washed with 50 ml tap water, then dried in a 50°C oven overnight.

4.3 Results and Discussion

4.3.1 The composition of wheat brans

Table 4.1 shows the composition of the seven wheat brans. The water extractable arabinoxylans (WEAX) in the 4% bran and the whole wheat bran were negligible (~ 2% of the dry weight of wheat bran). Thus the remaining extraction experiments were carried out omitting the extraction of WEAX. The total AX concentrations of 15-27% are lower than the value of around 30% typically suggested as the AX content of wheat bran (Maes and Delcour, 2001, 2002), due to most of the bran samples being diluted with starch.

The results from Table 4.1 indicate that as the level of pearling increased, both protein and starch content increased, while AX content decreased due to dilution from endosperm material removed by pearling. The starch, protein and AX contents of the bran produced by the Bühler milling were relatively unaffected by pearling, suggesting that preferential removal of the outer layers of the wheat kernels did not affect the gross composition of the remaining bran sufficiently to be detectable.

The most dramatic result from Table 4.1 is the high alkali-extractable arabinoxylans (AEAX) content of the bran produced by pearling to a level of 4%. This bran contained nearly 27% AX, 50% more than the bran produced by conventional milling of whole wheat. All of the other bran samples contained much lower AX levels, in the range of around 15-19% with no large differences or apparent trends. This result suggests strongly that obtaining bran by pearling to a level of around 4% would give high levels of AX for subsequent extraction. This is supported by the findings of Barron *et al.* (2007), who reported that arabinose and xylose (and by implication, AX) were more concentrated in the outer bran layers of two wheat varieties. Of course, the functionality of this AX compared with that occurring in other parts of the wheat kernel, or from other wheats, cannot be assumed; further work would be needed to investigate the relative functionalities of AX from different parts of the wheat kernel and from a wide range of wheats. The high content is also of benefit only if it actually leads to greater yields on extraction. This is investigated in the next section.

Table 4.1. The composition of the seven wheat brans produced from Consort wheat.

Compositions	Brans produced with a debranner			Bühler milled bran from whole wheat	Bühler milled brans from pearled wheat		
	4%	8%	12 %		4%	8%	12 %
Moisture (%, wet basis)	10.1	12.4	13.4	12.9	13.4	13.4	13.3
Protein (%, dry basis)	6.8	11.8	14.7	15.3	19.3	23.4	18.9
Starch (%, dry basis)	17.6	26.9	36.6	19.7	21.9	21.8	25.0
Glucose (%, dry basis)	3.1	3.4	3.3	3.5	3.7	3.2	3.3
Ash (%, dry basis)	2.8	1.8	1.9	5.4	4.9	5.3	5.5
Arabinoxylans* (%, dry basis)	26.8	18.6	16.0	17.7	17.2	15.8	17.1
Water extractable arabinoxylans (%, dry basis)	2.2	–	–	1.9	–	–	–
Arabinose (%, dry basis)	13.2	10.1	8.6	8.0	7.9	7.2	7.0
Xylose (%, dry basis)	17.2	11.1	9.5	12.1	11.6	10.7	12.4
A/X ratio	0.77	0.91	0.91	0.66	0.68	0.67	0.56
Others (%, dry basis)	37.1	34.9	25.4	34.1	30.7	28.4	27.9

* Arabinoxylans=0.88×(Arabinose+Xylose).

4.3.2 Arabinoxylan extraction from bran samples

The method described above was used to extract AX from the seven bran samples. For the preliminary work, the enzyme purification processes were omitted, such that only relatively crude and impure extracts were obtained. Figure 4.1 shows the results in terms of the yield and the purity (*i.e.* the AX contents of the extracts) of the crude extracts, and the absolute yield of AX (= yield × purity). For the bran produced by Bühler milling of whole wheat, the yield was about 11 g of extract from 50 g (wet basis) of bran, giving a dry basis yield of 25.3%. The AX content of this extract was around 42%. The other Bühler-milled bran samples gave similar yields but of lower purity. The highest yield, purity and absolute yield came from the bran obtained by pearling to 4% (labelled "4%P"); this was in line with expectations, as this bran had featured the highest AX content. The brans obtained from pearling to higher levels gave slightly lower purities and substantially lower yields, in line with their lower AX contents. These results confirm that AX appears to be more concentrated in the outer bran layers of the wheat kernel, and that obtaining bran for AX extraction by pearling to around 4% offers advantages in terms of the AX concentration of the bran. This assumes that this AX proves to have acceptable quality and functionality compared with AX from elsewhere in the wheat kernel. The higher AX content of bran pearled from the outer layers would also need to be confirmed for a wider range of wheats. In addition, the practicalities of handling the fine bran powder produced by pearling would need to be investigated.

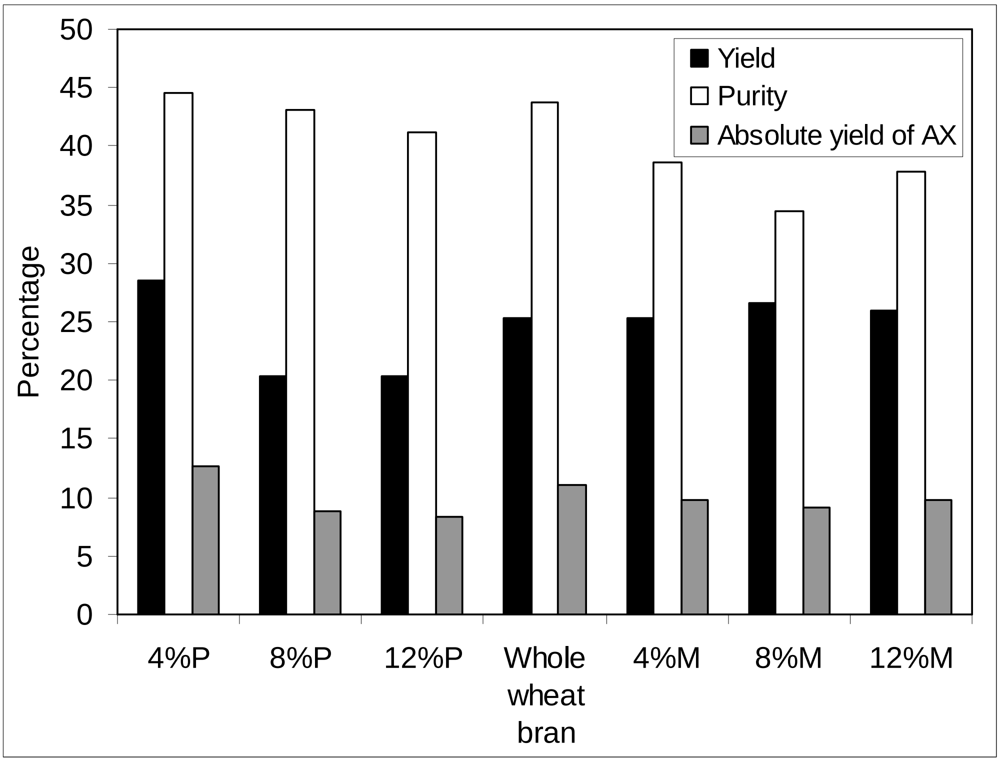


Figure 4.1. The yield, purity and absolute yield of AEAX products (dry basis).

4.3.3 Enzyme treatment of arabinoxylan extract

To further improve the purity of AX extracted from the 4% pearled bran, experiments were carried out with the enzyme treatment process. As shown in Table 4.2, with the enzymatic removal of protein, β-glucan and other impurities, the purity of AX in the crude powder was enhanced from 44.5% to 66.4%, while the yield of crude AX product decreased from 28.6% to 18.3%. The similar absolute yields of 12.7 and 12.1% confirm that the enzyme treatment process did not lead to significant losses of AX. Given that the 4% pearled bran initially contained 26.8% AX, around 46% of this was recovered.

Table 4.2. Comparison of the AEAX extraction process with and without enzyme treatment process from the 4% wheat bran (wb = wet basis, db = dry basis).

	AEAX without enzyme treatment process	AEAX with enzyme treatment process
Sample added (g, wb)	50	50
Moisture of sample (%wb)	10.1	10.1
Crude extract yield (g, db)	12.8	8.2
Yield of crude AX product (%db)	28.6	18.3
AX content of crude extract (%db)	44.5	66.4
Absolute yield of AX (=yield×purity, %db)	12.7	12.1
Arabinose concentration in products (%db)	23.9	32.7
Xylose concentration in products (%db)	26.7	42.8
A/X ratio	0.90	0.76

4.3.4 Starch recovery by water washing

The initial starch content in various wheat brans ranged from 18% to 37% (dry basis). To improve the economic performance of bioethanol plant, the starch should be recovered from the bran prior to AX extraction and sent back to the saccharification unit. Table 4.3 lists the starch contents of the seven different wheat brans before and after water washing pre-treatment. It indicates that more than 70% of the starch in the bran stream could be recovered by washing. However, some AX was lost during the removal of starch. Assuming that an optimised industrial operation would be at least as effective as this simple process, a level of starch recovery of 75% was assumed for the subsequent simulations of the ethanol-AX co-production process.

Table 4.3. Starch content and recovery ratio in water washing pre-treatment.

	Brans produced with a debranner			Whole wheat bran	Bühler milled brans from pearled wheat		
	4%	8%	12 %		4%	8%	12 %
Starch concentration before washing (%db)	17.6	26.9	36.6	19.7	21.9	21.8	25.0
Starch concentration after washing (%db)	5.8	7.8	16.7	6.8	9	8.5	11.5
Starch recovery ratio (%, g/g)	71.2	77.3	74.2	71.4	77.1	77.0	76.4

4.4 Conclusions

Bran samples were prepared by pearling wheat to 4, 8 and 12% of the initial wheat weight to recover bran, and by Bühler milling whole and pearled wheat. The AX content of bran recovered by pearling wheat to a level of 4% of the initial weight of the wheat, and the yield and purity of AX extracted from this bran, were greater than for the other brans. This suggests that AX is more concentrated in the outer layers of the wheat kernel, and that recovery of bran for AX extraction by pearling would give advantages in terms of yield. These results need to be confirmed for other wheats, and the practicalities of handling and processing of the fine bran powder produced by pearling investigated. In addition, the quality and functionality of the AX extracted from the outer bran payers, compared with AX arising from other parts of the wheat kernel, needs to be investigated.

Enzyme treatment of AX extracts significantly enhanced the purity of the extracts. The highest purity achieved in this brief study was 66%, with an absolute yield of AX of around 12% of the initial dry weight of the bran, or just under half of the initial AX present in the bran.

Washing bran with water resulted in a 71-77% starch recovery for return to the ethanol production section.

5. Simulation of co-production of ethanol and arabinoxylan

5.1 Introduction

The work presented in the previous chapters concluded that AX extraction in the context of a bioethanol plant appeared economically feasible, that the use of debranning to obtain bran offered several advantages, but that recovery of bran after hammer milling might be cheaper. These two options were therefore analysed further by conducting full simulations using SuperPro Designer. The base case of wheat-to-ethanol-plus-DDGS was also simulated.

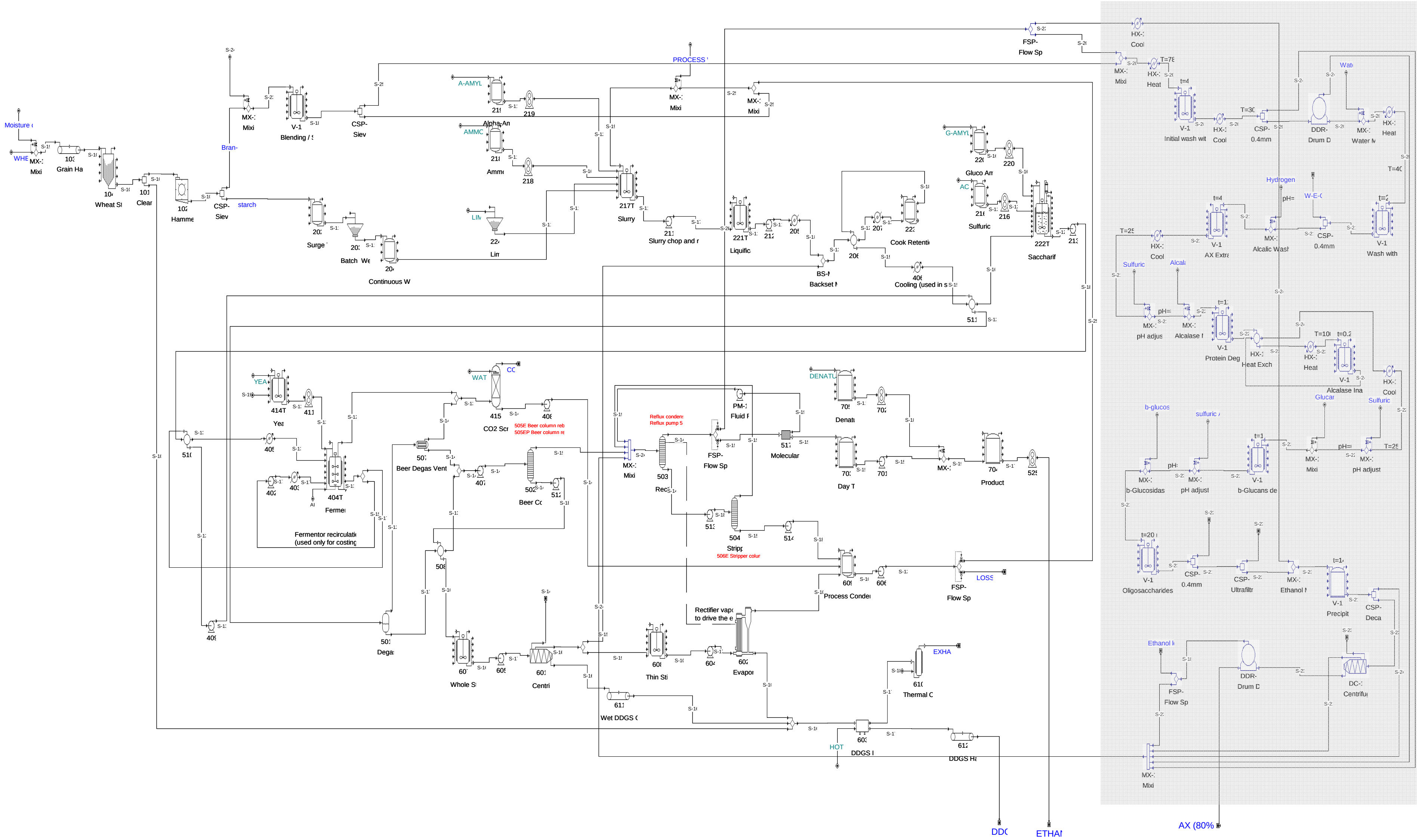
This chapter presents full simulations of ethanol production with and without AX extraction from bran, with bran obtained either by hammer milling and sieving, or by debranning. The flowsheets are firstly defined in detail. The parameters considered for capital cost and operating cost estimation (including raw materials, utilities, labour and facility-dependent costs), and the bases for these costs estimates, are then detailed. The results are considered in terms of the contributions of the various revenue streams and cost components, and the production costs of an AX product of 80% purity in order to give the same return on investment (ROI) as the base case. Sensitivity analyses and consideration of possible process improvements are presented. Finally conclusions are drawn regarding the feasibility of incorporating AX extraction into ethanol production from wheat, and regarding the further research required to enable such a prospect to be implemented effectively.

Throughout this chapter, in common with the general convention of published literature on studies of process economics, costs are presented in US$. However, the most basic costs like the cost of wheat and utilities were set according to their relevant UK prices. The ratio of \$2 = £1 was used throughout. Costs have been converted back to £ for the purposes of final presentation and discussion.

5.2. Flow diagram development and economic evaluation of AX extraction

This section develops a flow diagram of the process. It considers the industrial equipment suitable for up-scaling the process and suggests the characteristic parameters of each procedure according to data from Hollmann and Lindhauer (2005). The process is simulated using SuperPro Designer (Intelligen Inc., MIT). Figure 5.1 shows the integrated flowsheet that was developed based on the proposals of Maes and Delcour (2001) and Hollmann and Lindhauer (2005). Once the technological part of the project is established, the capital and operating costs of the process are considered in order to allow estimation of the production costs.

Figure 5.1. Flowsheet of the integrated AX co-production section within a wheat-to-ethanol plant. Bioethanol flowsheet structure and costs adapted from Kwiatkowski *et al.* (2006). AX co-production section adapted from Hollmann and Lindhauer (2005).



5.2.1. Flow diagram explanation

The AX extraction process was integrated within a typical bioethanol plant. The structure of the bioethanol plant was adapted from Kwiatkowski *et al.* (2006), who modelled a typical dry-grind corn-to-ethanol process using SuperPro Designer. In order to convert the corn-to-ethanol to wheat-to-ethanol plant some essential changes have been made for achieving the yields of a typical equivalent process, as described in Chapter 2. Figure 5.2 shows the overall yields that the simulation was based on (Mortimer *et al.*, 2004). The base case wheat-to-ethanol plant has a capacity of about 102 million kg of ethanol per annum. The ethanol is to be used as a fuel additive, allowing for petrol to be used as denaturant at a final concentration about 4.4%. The ethanol concentration of the broth is 8.5% and it is distilled up to 93.5%. The overall yield, based on starch, of the wheat-to-ethanol process is less than the typical corn-to-ethanol process, resulting in relatively more DDGS, about 1.45 tonnes for every tonne of bioethanol produced (Mortimer *et al.*, 2004).

Two AX co-production scenarios were developed. In the first the wheat is hammer milled and sieved. The bran particles larger than 0.5 mm (assumed to represent 4.4% of the total wheat) are passed to the AX co-production section. In the second scenario the wheat is debranned up to 4.4% and the bran powder is sent to the AX co-production section. These percentages were chosen in order to give a bran-rich stream with a flowrate of about 2 t/h.

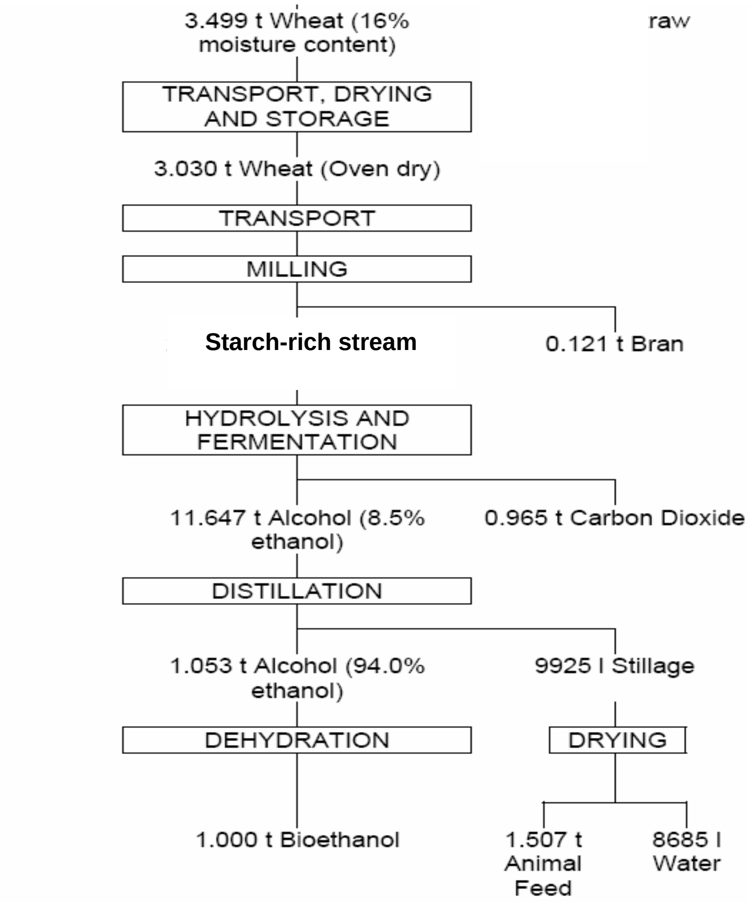


Figure 5.2. The wheat-to-ethanol base case yields (adapted from Mortimer *et al.*, 2004).

5.2.1.1. Process description

Referring to Figure 5.1 and to Hollmann and Lindhauer (2005), the AX production section was integrated within the base case wheat-to-ethanol flowsheet. The by-product of wheat milling, bran (particle size larger than 0.5 mm), is initially washed with 70% ethanol, up to a final concentration of 60% ethanol. The purpose of the initial wash is to extract low molecular weight contaminants such as fat, vitamins and other impurities, and to inactivate the arabinoxylan-degrading enzymes that naturally exist in the bran. The mixture is heated to 80°C for 4 hours, in the first jacketed tank with continuous stirring, and then cooled to 30°C. The fat-free bran is collected with a 0.4 mm sieve and then dried in a vacuum drum dryer, to recover all the ethanol that was previously added.

The second purification step involves the separation of the water-extractable arabinoxylans (WEAX) and part of the β-glucans. The fat-free bran is suspended in water and heated to 40°C for 2 hours, in the second jacketed tank with continuous stirring. The water to fat-free bran mass ratio is 11.6, corresponding to a bran concentration of 8%. The bran is then collected on a 0.4 mm sieve.

The purified WEAX-free bran is then treated in the main step of the AX extraction. The proposed conditions are 40°C for 4 hours with continuous stirring, suspended in 2% hydrogen peroxide solution, for which the pH value has been adjusted to 11 with 25% sodium hydroxide. The bran concentration is about 5%. During the alkalic wash AX, protein, cellulose, starch and β-glucans are extracted, each one with different percentages. However, the specified conditions are highly selective for the AX (Maes and Delcour, 2001; Hollmann and Lindhauer, 2005).

After the extraction, proteins and β-glucans are removed enzymatically. The mixture is cooled to 25°C which is the optimum temperature for alcalase (protease) treatment, and the pH value is adjusted to 8.5 with 25% sulphuric acid. Alcalase is added and the mixture is continuously stirred in a jacketed tank for 12 h. The suspension is then heated to 100°C for 10 minutes in a jacketed tank, for the inactivation of the alcalase, and then cooled to room temperature.

The suspension is then treated with lichenase for the degradation of β-glucans. The pH value is adjusted to 6.5 with 25% sulphuric acid and after the addition of lichenase the mixture is held for 1 hour in a jacketed tank with continuous stirring. Then the pH value is adjusted to 4, with 25% sulphuric acid, and β-glucosidase is added. After 20 minutes of continuous stirring in a jacketed tank, the bran particles are collected on a 0.4 mm sieve, and the filtrate is concentrated with ultrafiltration, in order to reduce the ethanol requirement at the precipitation step.

The next step involves the precipitation of the AX. 96% ethanol is added, up to a final ethanol concentration of 65%, and the mixture is loaded in a tank without stirring, for 14 hours. The precipitated AX is then sent in a decanter centrifuge, from which it is collected and dried in a drum dryer.

All the output streams that contain ethanol from the several steps are recycled to the bioethanol processing section. Their ethanol concentration is about 70% and so they can be added directly to the rectifier column. The recycling affects the sizes of both the rectifier and the stripping columns. The losses of ethanol in the AX co-production section loop were assumed to be 2%.

5.2.1.2. Scaling up differences and assumptions

The industrial process will have some differences compared with the one developed at the laboratory scale. In the following paragraphs, each difference is analysed and explained. In addition, several details and assumptions are analysed.

The starch loss in the bran-rich stream is a very important aspect that will reduce the overall ethanol yield. The wheat bran used in the paper of Hollmann and Lindhauer (2005) was previously destarched without the researchers indicating the details of the process. The initial starch concentration of their bran was 8.5%, when the starch concentration of a bran-rich stream produced by short flow roller milling or recovered by debranning might be as much as 20% (see Table 4.1). Several destarching techniques are available in the literature. One of them is the one applied in wet-milling corn-to-ethanol processes, in which the grains are steeped in a H_2SO_3 solution (2000 ppm SO_2) for 24-48 hours. The SO_2 releases the bonds between starch and proteins, making the starch available to be recovered (Rausch and Belyea, 2006). From the results presented in the previous chapter, it appears that a simple wash with water is able to recover more than 70% of the starch initially existing in the bran-rich stream of both the whole wheat bran and the bran recovered by pearling to 4%. An equivalent washing with water is applied later to the second purification step; however a wash with water immediately after sifting was also considered. The starch recovered, along with the additional quantity of water, is then used in the liquefaction stage of the ethanol production section. The total starch losses to the bran-rich stream (assuming an initial 16% starch content in the 4.4% bran removed) are less than 1%, 75% of which is recycled and sent to the liquefaction tank, while the remainder is lost to the AX production stream. Part of this lost starch ends up in the waste streams following washing (due to the several washings in the AX production), part is hydrolysed (due to the enzymatic treatments), and part of the starch is present in the final AX product.

In the suggested process as stated in the paper of Hollmann and Lindhauer (2005), the bran particles were dried prior the third wash with alkaline H_2O_2, immediately after the second sieving, as shown in Figure 5.1. In an equivalent industrial process, this second drying could be omitted. The wet bran particles could be collected by the sieve and directly passed to the third wash. However, the first drying operation after the 65% ethanol wash was included in the simulation. The main purpose was the recovery of the solvent. The wet bran particles collected by the several sieves after the washing steps were assumed always to have about 50-60% moisture. When the solvent was ethanol-water mixtures, it was assumed that the wet bran particles will contain, in proportion with the initial mixture, amounts of ethanol and water up to a concentration of 50-60%.

It was assumed that all the macromolecules contained in the wheat bran have the same thermophysical properties as glucose. The properties that would theoretically affect the economic result are their heat capacity and density.

One of the basic differences of the two scenarios is the particle size of the bran produced by the two different milling operations. In the first flowsheet only the coarse particles are led to the AX co-production section. This fact allows the removal of the particles after each washing step by only using a sieve that has smaller openings than the bran particles. The majority of the solvents are removed without having additional energy requirements. In the second alternative the finer bran powder produced by the debranner probably does not allow the same simple operation to be employed. Even if the same sieving technology is used, by choosing a sieve with smaller openings, it is expected that the losses will affect the overall yield.

There are plenty of available technologies for dewatering of a suspension without excessive energy requirements. It is not expected that the differences will be dramatic. However, both capital and energy requirements for processing fine bran powder are conservatively considered in the current work.

5.2.2. Parameters for Capital Costs estimation

As noted above, in common with most process economic evaluations in the public domain, all the costs provided in this work are given in US$, although costs are selected as much as possible to be relevant to the UK context. The ratio of $2 = £1 was used in all cases. Final costs are presented in £.

The process was evaluated for a 10 year project life time, assuming the plant to be operational for 330 days per year. The bran flowrate that is passed to the AX production section is 2 t/h with a 7% moisture content. The construction year was assumed to be 2007, with a construction period of 6 months.

The process is divided into the following sections:

1. Grain handling and milling
2. Starch to sugar conversion
3. Fermentation
4. Ethanol processing
5. Co-product processing
6. AX-co-production

The structure of the first five sections and the models for the cost estimation were set according to Kwiatkowski *et al.* (2006). The models for the cost estimation of the major equipment of the AX production section are as follows:

Jacketed Tanks

All the tanks shown in the flow diagram are jacketed tanks with an agitator, apart from the last one in which precipitation takes place, which does not include an agitator. The equation used to calculate the cost of the tanks, is:

$$\text{Cost} = C_0\left(\frac{Q}{Q_0}\right)^a \qquad (5.1)$$

where Q is the size of the tank in m^3, Q_0 is the reference size, 30 m^3, C_0 is the reference cost which was $27300 in 1998 (Loh and Lyons, 2002) and a is the cost capacity exponent which is 0.55 for tanks (Peters *et al.*, 2003). All tanks are assumed to be constructed from carbon steel except tanks identified as V-103, and V-107 in Figure 5.1. In tank V-103 the AX extraction takes place with a pH value 11, and in V-107 the enzymatic treatment takes place with β-glucosidase at pH 4. The pH values are relatively extreme, and so stainless steel is suggested for their construction. The costing equation was calculated for carbon steel, and so the material factor is 0 for all tanks, except V-103 and V-107 for which the material factor is an accumulative 0.9 for stainless steel 304 that will be used. The installation and maintenance factors are 0.5 and 0.1, respectively (Peters *et al.*, 2003).

Heat exchangers

The cost of the heat exchangers used for cooling and heating was estimated by Equation 5.1, with Q being the size of the exchanger in m^2, Q_0 the reference size, 9.5 m^2, C_0 the reference cost which was \$13200 in 1998 (Loh and Lyons, 2002) and the cost capacity exponent a=0.9. All heat exchangers are shell and tube and constructed from carbon steel. The installation and maintenance factors are 0.5 and 0.1, respectively (Peters *et al.,* 2003).

Sieves

The sieves where assumed to be rotary drum 0.4 mm screens with a total drum surface 5.2 m^2 (Anonymous, 2006a). The construction material is carbon steel and the purchased cost was estimated to be \$26200. The last sieve, P-14, is made from stainless steel and its cost is estimated to be \$31500 (Anonymous, 2006a). In all cases the installation and the maintenance factors are 0.7 and 0.2, respectively (Peters *et al.*, 2003).

Vacuum Drum Dryers

Drum dryers were assumed for the drying operation, because of their frequent use when cereals are processed, although there are cheaper solutions such as air dryers. The selected drum dryers operate under vacuum for the recovery of the ethanol. For the vacuum drum dryers the capacity is measured in m^2 and represents the drum's surface area. The base capacity is 23.5 m^2, with a cost of \$650000 and the cost capacity exponent is 0.6 (Peters *et al.,* 2003). Installation and maintenance factors are 0.5 and 0.1, respectively.

Because of the uncertainty of the cost capacity exponent at extreme sizes of each piece of equipment, the values of some very small or very large tanks and heat exchangers were set by slightly modifying some of the models. In such circumstances, the models were developed for every kind of equipment using tables with the exact costs (Loh and Lyons, 2002). Appendix C shows the exact size and the exact purchase cost of each unit of the flow diagram.

For the estimation of the Direct Fixed Capital (DFC) the several items are proportional with the total delivered equipment purchase cost. The ratio factors of piping, instrumentation *etc.* of the bioethanol production were set according to Kwiatkowski *et al.* (2006). Table 5.1 shows the equivalent factors for the integrated AX production section. The cost of the unlisted equipment was assumed to be 5% of the purchased cost of the listed equipment, with an installation factor 0.5. It includes the necessary pumps, valves and drivers.

The installation factor was set to each unit individually since it varies depending on the kind of equipment and a typical value wouldn't be adequately representative. The construction material factors were set to zero, since the purchased costs were estimated for carbon steel construction, apart from the units constructed in stainless steel 304, which has a factor of 0.9.

Other capital costs include the steam generation, cooling water generation, Clean-In-Place and wastewater treatment equipment. Their contribution is about \$3.3 million (Kwiatkowski *et al.,* 2006). Having all the above data, the DFC can now be estimated.

The working capital was assumed to be \$200000. The start-up and validation costs were set at 5% of the DFC (Peters *et al.,* 2003). The up-front Research and Development and the up-front Royalties were assumed to be zero. By accumulating the latter values to the DFC, the Total Capital Investment can be estimated.

Table 5.1. Ratio factors for estimating the Direct Fixed Capital.

Direct costs		Bioethanol[a]	***AX production*** [b]
1	Installation	Was set individually	
2	Process Piping	0.25	0.31
3	Instrumentation	0.20	0.26
4	Insulation	0.03	0.03
5	Electrical systems	0.15	0.10
6	Buildings	0.20	0.30
7	Yard Improvement	0.02	0.12
8	Auxiliary Facilities	0.10	0.55
Indirect costs			
9	Engineering	0.32	0.32
10	Construction	0.34	0.61
Other costs			
11	Contractor's fee	0.00	0.19
12	Contingency	0.06	0.37

[a] Kwiatkowski *et al.* (2006) for bioethanol
[b] Peters *et al.* (2003) for the AX co-production section

5.2.3. Parameters for Operating Costs estimation

The major components of the operating costs are:

1. Raw materials costs
2. Utilities costs
3. Labour costs
4. Facility-dependent costs (*e.g.* depreciation, maintenance, and facility-dependent miscellaneous such as insurance, local taxes and other factory expenses)
5. Miscellaneous costs (research and development, process validation, and royalties throughout the life time of the plant).

5.2.3.1 Raw materials

The raw materials of the first five sections (the bioethanol production) were set according to Kwiatkowski *et al.* (2006). The price of wheat was assumed to be \$200 per tonne (£100 /tonne). The required amounts of the raw materials used for the AX co-production section were estimated from data provided by the paper of Hollmann and Lindhauer (2005). Table 5.2 summarises the required annual amount and the cost on a \$/kg basis of each raw material.

Table 5.2. Raw materials costs.

Bulk Raw Material	**Unit Cost (\$/kg)**	**Reference**	**Annual Amount (kg)**
Wheat	0.200		311652000
Water	0.000044	Kwiatkowski *et al.*, 2006	644172443
Lime	0.090	Kwiatkowski *et al.*, 2006	424583
Liquid Ammonia	0.220	Kwiatkowski *et al.*, 2006	710606
Alpha-Amylase	3.310	Kwiatkowski *et al.*, 2006	249155
Gluco-Amylase	3.310	Kwiatkowski *et al.*, 2006	359877
Sulphuric Acid	0.110	Kwiatkowski *et al.*, 2006	2428621
Yeast	5.510	Kwiatkowski *et al.*, 2006	86645
Octane	0.200	Kwiatkowski *et al.*, 2006	4516457
Hydrogen Peroxide	1.100	Anonymous, 2006	4122682
Alcalase	61.000	L Clabby, 2006[a]	9161
Glucanase	52.600	L Clabby, 2006[a]	9254
β-Glucosidase	42.400	L Clabby, 2006[a]	9348

[a] personal communication

5.2.3.2. Utilities

Table 5.3 shows the costs of the utilities. These costs are typical costs for the UK context (even though they are shown in US\$). The electricity consumption was set for each operating unit individually. The additional electricity general load of the AX co-production section (which includes lighting, monitoring devices *etc.*) was assumed to be 15% of the total load required. The electricity requirements of the unlisted equipment (pumps, conveyors) were assumed to be 5% of the total (Peters *et al.*, 2003).

Table 5.3. Utilities costs.

Utilities	**Cost**	**Unit**
Electricity	0.08	$/kWh
Heat transfer agents		
Cooling Water	0.07	$/tonne
Chilled Water	0.4	$/tonne
Steam	17	$/tonne
Natural Gas	289 (or 5.65)	$/tonne (or $/GJ)

5.2.3.3. Labour costs

The labour costs were estimated by accumulating the operator hours per operating hour ratios. Data for the labour requirements of each operation unit are shown in Table 5.4 (Peters *et al*., 2003). The labour costs were estimated assuming a basic labour rate 15 $/h. The labour-dependent miscellaneous costs categorised in 5.2.3. include the Laboratory, Quality Control (QA) and Quality Assurance (QC) costs. Their sum was set to 15% of the total labour (Peters *et al.,* 2003) for the AX section and zero for the overall bioethanol section, since it is not a product that requires substantial QC or QA.

Table 5.4. Labour requirements analysis.

	Workers/unit/shift
Tank	0.4
Sieve	–
Drum	0.5
Heat exchangers	0.1
Ultrafiltration	0.5
Decanter/Centrifuge	0.5
Total	5.6
Fringe benefits	40% of total
Supervision	15% of total
Operating Supplies	10% of total
Administration	60% of total

5.2.3.4. Facility-Dependent Costs

The facility-dependent costs include the following items:

- Depreciation. The Total Capital Investment is annualised depending on the project life time. Additional expenses for interest are also charged.
- Maintenance costs: The equipment maintenance costs on an annual basis were set according to specific multipliers for each kind of equipment within the range 0.1-0.3 of the Purchased Cost (Peters *et al.,* 2003).
- Miscellaneous: Insurance (1% of the DFC), Local taxes (2% of the DFC), other factory expenses (5%) (Peters *et al.,* 2003).

5.2.4 Results of the economic evaluation

Usually techno-economical reports also include market research in order to estimate a competitive selling price for the products. The suggested selling price is then set in order to reach conclusions about the economic potential of the selected technology or whether it is worthy to produce the product. However, since there is no market for AX at the moment or a commercial source with a specified price, this research instead takes the approach of estimating the production cost based on a minimum acceptable economic result – in this case, the return on investment for the plant.

Co-production of AX was considered under two scenarios as described above: AX extracted from large bran particles recovered from hammer milling, and AX recovered from fine bran particles obtained by debranning. In the following paragraphs, the first scenario is called "AX co-production" and the second is called "AX from 4.4% debranning".

In order to estimate the AX production cost under the two alternatives, the following technique was used. The costs and the revenues of the base case wheat-to-ethanol-plus-DDGS plant were first estimated. The selling price of DDGS was set at 0.1 $/kg in all cases. The economic criterion that was chosen for the comparison was the Return On Investment (ROI = Net Profit/Total Investment), which is inversely proportional to the payback time (the time required for the depreciation of the total investment), this being is the most commonly used criterion for the economic performance of a plant (Zutter, 2007). To achieve an acceptable ROI of about 17% (corresponding to a payback time of about 6 years), the selling price of ethanol had to be 0.71 $/kg (with income taxes set at 40% in all cases). This value was set as the ethanol selling price for both of the AX co-production alternatives considered in the current work.

The impact of the integration of the AX co-production section is to reduce the revenue of both of the original product streams, ethanol and DDGS. The production of ethanol is lowered due to losses of starch to the bran-rich stream and losses of ethanol used in the AX extraction process. The overall reduction of the final ethanol production is 2.5% for both AX co-production alternatives, while DDGS production is reduced by 8%. Figure 5.3 shows the differences of the flowrates of the revenue streams. In both the AX co-production alternatives the annual AX production is about 2.18 million kg.

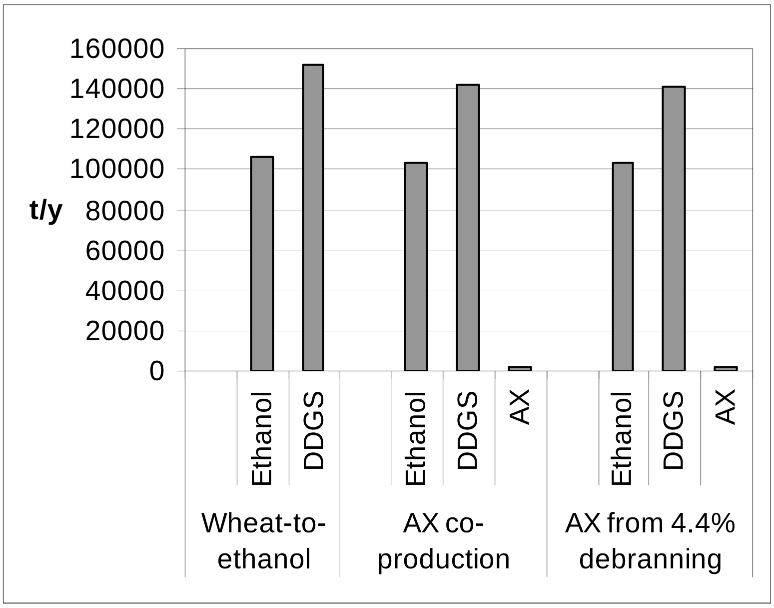


Figure 5.3. Flowrates of the revenue streams.

As shown in Appendix C, the DFC of the first five sections (bioethanol production) is slightly decreased (0.2%). This arises because of the lowering of the flowrate of the starch-rich stream, hence requiring slightly smaller and cheaper equipment. The DFC of the AX production section was estimated to be about $10 million for the initial hammer milling and $16 million for the debranning alternative. Table 5.5 shows the DFC of each section of each flowsheet.

Table 5.5. DFC of the sections of each flowsheet.

	Wheat-to-ethanol [a]	AX co-production	AX co-production by debranning
Grain handling and milling	3,197,000	3,182,000	3,175,000
Starch-to-sugar conversion	6,589,000	6,550,000	6,037,000
Fermentation	12,092,000	11,987,000	12,127,000
Ethanol processing	8,173,000	8,321,000	8,118,000
Co-product processing	20,597,000	20,502,000	20,506,000
Common support systems	600,000	600,000	600,000
AX co-production	–	10,183,000	15,936,000
Total DFC	**$51,248,000**	**$61,326,000**	**$66,498,000**

[a] adapted from Kwiatkowski *et al.* (2006)

The difference of the DFC between the two AX-producing flowsheets occurs firstly because of the cost of the debranner and secondly because of the fine bran powder that it produces. Due to lack of data for the estimation of the debranner's purchase cost, an expensive $1 million was assumed. The debranner's installed contribution to the DFC of the AX production section is then more than $3.5 million. Furthermore, several other changes contribute to the difference. The fine bran powder from the debranner requires more complex operating units in order to be recovered after each washing operation. In the absence of experimental studies, it is not clear whether a simple rotating sieve would be able to recover the fine particles without significant losses. A conservative assumption increases the costs of the filtrations. In addition, the moisture content of the particles is likely to be larger than the 50-60% that was assumed for the initial flowsheet, as the smaller particles will drain less readily. Assuming the moisture to be about 60-70% the size of the dryers required to dry the bran particles is larger, adding to the DFC costs.

The raw material costs are also increased in both the AX co-production alternatives. Table 5.6 shows the raw material annual costs of each flowsheet. It highlights the additional raw materials costs required for the AX co-production. It should be noted that it considers their contribution to the overall plant, a break down within the AX section is given later. Table 5.7 shows the utilities, the labour and the labour-dependent miscellaneous (laboratory, QC, QA) annual operating costs. It then provides the facility-dependent costs, which as mentioned in section 5.2.3.4 include depreciation (10 years, linear, assuming the interest to be 7%), maintenance and facility-dependent miscellaneous (local taxes, insurance *etc.*).

Table 5.6. Raw materials annual costs of each flowsheet (numbers in brackets indicate the percentage each raw material contributes to the total raw material costs.

Bulk Raw Material	Wheat-to-ethanol [a]	AX co-production	AX co-production by debranning
Wheat	62,330,000 (94.40%)	62,330,000 (86.16%)	62,330,000 (85.68%)
Glucoamylase	1,191,000 (1.80%)	1,191,000 (1.65%)	1,191,000 (1.64%)
Octane	925,000 (1.40%)	902,000 (1.24%)	900,000 (1.23%)
Alpha-Amylase	825,000 (1.25%)	825,000 (1.14%)	825,000 (1.13%)
Yeast	477,000 (0.72%)	477,000 (0.66%)	477,000 (0.65%)
Ammonia	156,000 (0.23%)	156,000 (0.21%)	156,000 (0.21%)
Sulphuric Acid	78,000 (0.12%)	78,000 (0.11%)	78,000 (0.11%)
Lime	38,000 (0.06%)	38,000 (0.05%)	38,000 (0.05%)
Water	9,000 (0.01%)	9,000 (0.01%)	9,000 (0.05%)
SUB-TOTAL FOR ETHANOL	**66,031,000 (100%)**	**66,006,000 (91.24%)**	**66,004,000 (90.68%)**
Hydrogen Peroxide	-	4,640,000 (6.4%)	4,916,000 (6.76%)
Alcalase	-	572,000 (0.79%)	629,000 (0.86%)
Glucanase	-	498,000 (0.69%)	548,000 (0.75%)
β-Glucosidase	-	406,000 (0.56%)	446,000 (0.61%)
Sulphuric Acid	-	194,000 (0.27%)	213,000 (0.29%)
Water	-	27,000 (0.04%)	26,000 (0.04)
SUB-TOTAL FOR AX ($/y)	**-**	**6,337,000 (8.76%)**	**6,778,000 (9.31%)**
TOTAL ($/y)	**66,031,000**	**72,343,000**	**72,782,000**

[a] adapted from Kwiatkowski *et al.* (2006)

Table 5.7. Utilities, labour, miscellaneous and facility-dependent annual costs.

	Wheat-to-ethanol [a]	AX co-production	AX co-production by debranning
Utilities	10,160,000	12,078,000	13,295,000
Labour	1,309,000	2,349,000	2,607,000
Miscellaneous	-	156,000	234,000
SUB-TOTAL ($/y)	11,469,000	14,583,000	16,136,000
Facility-dependent	7,364,000	9,466,000	10,561,000
TOTAL ($/y)	**18,833,000**	**24,049,000**	**26,697,000**

The largest contributors to the annual operating costs are the raw materials costs. Figure 5.4 breaks down the operating costs of the base case wheat-to-ethanol. The broken down operating costs of the two AX flowsheets are almost the same as the base case. Of the raw materials, the wheat comprises the predominant cost. Its cost represents about 95% of the total raw materials in the base case, and 86% for AX co-production. In the AX producing flowsheets, hydrogen peroxide accounts for about 5% of the overall operating costs and about 6.5% of the raw material costs.

Clearly, the addition of AX extraction has increased utilities costs substantially as a proportion of total costs, primarily because of the additional ethanol recovery by distillation, and because of additional steam, cooling water and electricity required in the AX co-production section for heating, drying, cooling and stirring of the tanks. The labour and the facility-dependent costs are also increased after the integration of the AX co-production section.

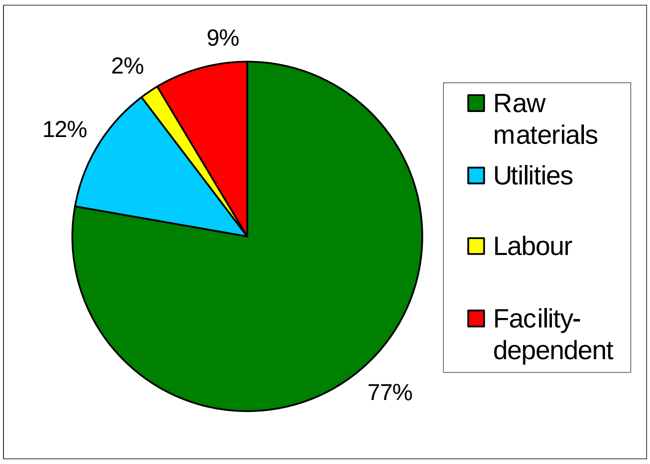


Figure 5.4. Break down of the Wheat-to-ethanol annual operating costs.

Table 5.8 summarises the costs and the revenues of the flowsheets, in order for the production cost of AX to be determined. In order to estimate the production cost of AX in the two flowsheets, the selling price of AX (80% purity) was set such that it will provide the same economic result with the base case flowsheet (ROI 17% or Payback Time about 6 years). The selling prices of ethanol and DDGS were kept constant at 0.71 and 0.1 $/kg, respectively. The AX production costs were found to be $7.3 (£3.65) and $9.1 (£4.55) per kg for the hammer milling and debranning alternatives, respectively.

Table 5.8. Profitability Analysis.

	Base case	AX co-production	AX co-production by debranning
TOTAL INVESTMENT ($)	51,248,000	62,035,000	67,495,000
TOTAL ANNUAL OPERATING COSTS ($/y)	**84,864,000**	**96,391,000**	**99,482,000**
REVENUES ETHANOL ($/y)	75,591,000	73,701,000	73,493,000
REVENUES DDGS ($/y)	15,219,000	14,003,000	14,014,000
REVENUES AX ($/y)	-	15,850,000	19,960,000
TOTAL ANNUAL REVENUES ($/y)	**90,810,000**	**103,553,000**	**107,466,000**
GROSS PROFIT ($/y) [a]	5,946,000	7,162,000	7,985,000
TAXES (40%)	2,378,000	2,865,000	3,194,000
NET PROFIT [b]	8,692,000	10,430,000	11,439,000
PAYBACK [c] TIME (y)	5.90	5.95	5.90

[a]: Total Revenues minus Total Operating Costs

[b]: Gross Profit minus Taxes plus Depreciation (it should be noted that the depreciation is not taxed, and is considered as revenue)

[c]: Net Profit divided by Total Investment

From a different perspective, the integration of the AX co-production within a wheat-to-ethanol plant requires a total investment of about $11.8 million (or £5.9 million) according to Flowsheet 2. The total annual operating costs are $11.5 million (or £5.75 million) more, including the annualised depreciation of the Total Investment. The revenues of ethanol and DDGS are reduced by about $3.1 millions (£1.55 million). The 80% purity AX product flowrate is 2.17 million kg per annum, and so the corresponding cost of production is about $6.72 /kg (£3.36 /kg). The additional $0.6 /kg of product (corresponding to an additional revenue $1.25 millions per annum or $750000 per annum after taxes) plus the depreciation of the section (about $1 million annually) are suitable to provide the equivalent 17% Return On (additional) Investment.

Figure 5.5 shows the cumulative revenues of the co-products of each flowsheet, highlighting the reduction of the revenues of ethanol and DDGS resulting from AX production. All these losses were charged to the AX production cost. It should also be remembered that the difference of the AX revenues in the alternative flowsheets occur only because the selling price of AX was fixed for achieving a constant economic result, and not because of differences in the quantities of AX produced; the annual production of AX in both flowsheets was the same (2171182 kg/annum).

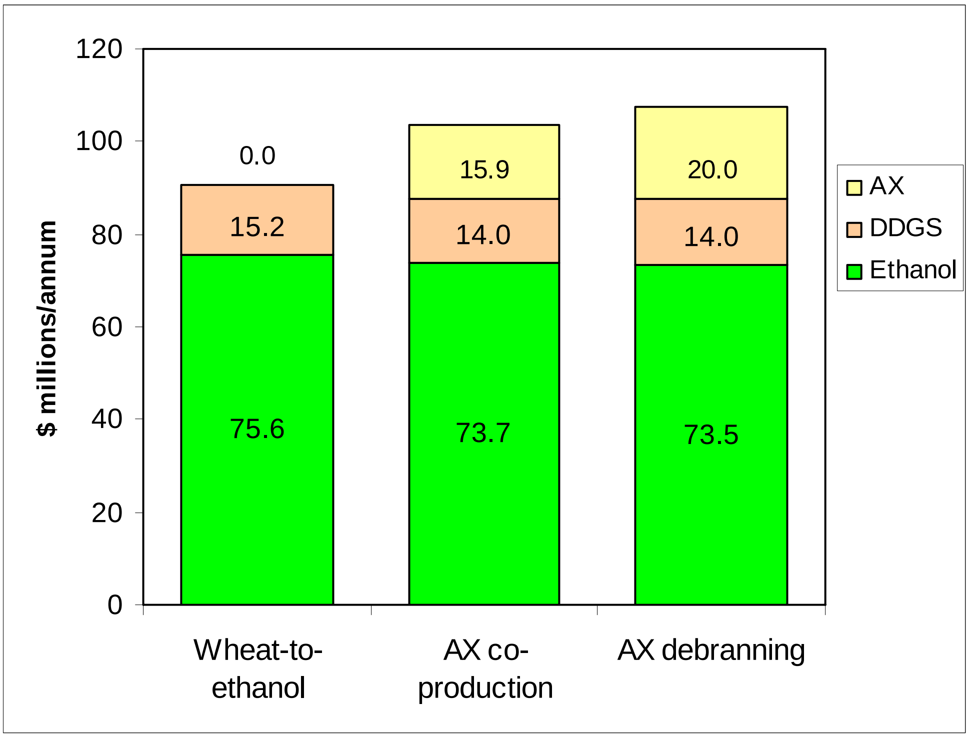


Figure 5.5. Cumulative revenues of each flowsheet
(price of AX set in order to achieve a payback time of six years).

Figure 5.6 shows the cumulative contribution of each cost for AX production. The raw materials include the reduced incomes due to lower ethanol and DDGS production. The raw materials represent 71% of the total cost. Hydrogen peroxide is the main contributor of the raw materials cost of AX, accounting for 2.14 $/kg of AX produced.

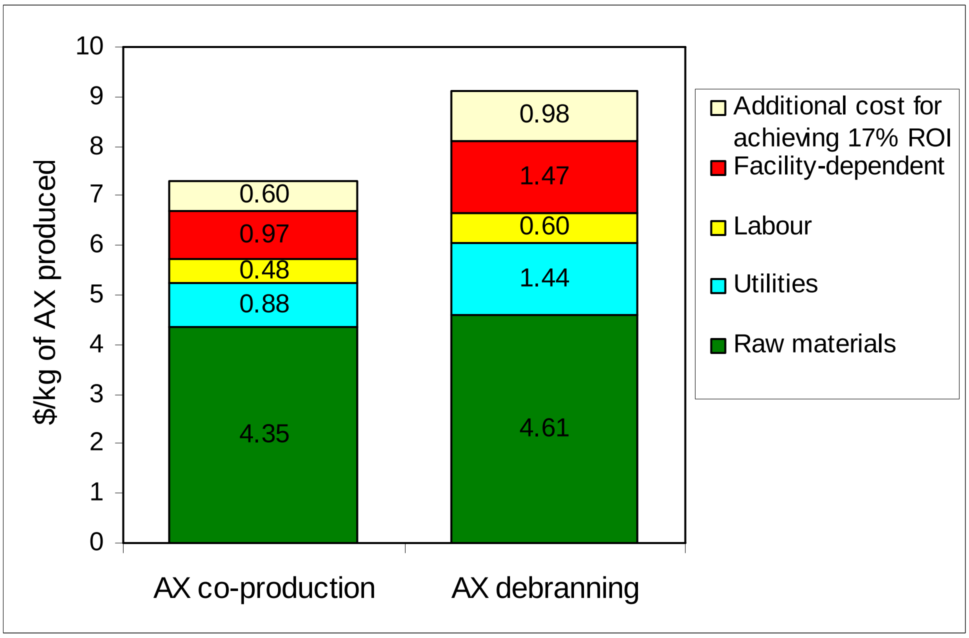


Figure 5.6. Cumulative contribution of each cost to the final AX price.

Clearly the AX co-production via debranning is more expensive. As already stated, this happens for the following reasons:

- Firstly, because of the assumption that the debranner itself costs \$1 million. The overall installed cost contribution of the debranner to the DFC in that flowsheet is more than \$3.5 million. A more accurate cost estimate, if lower, would reduce the estimate of the cost of AX produced by this route. Even so, halving this estimated cost did not alter the conclusion that AX production by this route was more expensive.
- Secondly, because it is assumed that the fine bran particles cannot be separated by a simple sieving operation after every washing. This results in more expensive dewatering equipment that requires more utilities. In addition it was assumed that the water content of the wet bran particles after every filtration is 60-70%. The steam consumption for heating and for the drum dryers is therefore larger. The electricity consumption of the debranner was set at 850 kW. The burden is reflected in the dramatic increase of the utility requirements shown in Table 5.7. With bran recovery from hammer milling, the additional utilities cost about \$1.9 million/y, while with the debranner, the additional utilities cost about \$3.15 million/y (65% more).

Debranning separates the outer layers, which it appears are more concentrated in AX. This major advantage wasn't allowed for in the current simulation; the bran composition was assumed to be the same for the two scenarios. The additional costs listed above might be offset by the higher concentration of AX in these outer layers, depending on its functionality. Until further laboratory research on AX extraction and functionality is undertaken, the debranning alternative cannot be completely ruled out. In addition, the suitability of cheaper dewatering techniques should be tested. However, for the remainder of the current research, only the first of the two AX extraction alternatives is considered for further evaluation and comparison with the base case.

5.2.5. Sensitivity Analysis

As already shown, the most important costs of the process are the raw material costs. It is necessary to perform a sensitivity analysis in order to estimate the prices of the co-products when the costs of major contributors are increased or decreased. The predominant factor is the cost of wheat.

However, it is difficult to predict or estimate the selling price of the DDGS in respect of the wheat price. In reality, the selling prices vary corresponding to changes of the basic raw material, but they are also dependent on the supply and demand of the market. Figure 5.7 shows the variation of the selling prices of the co-products of the corn-to-ethanol industry (Rausch and Belyea, 2006). It can be recognised that DDGS and ethanol prices are correlated, both being dependent on the price of corn. However, it can also be realised that there is a general downward trend in the market of DDGS, as a result of the increased supply over the last decade. It is believed that these trends will continue during the next decades (Rausch and Belyea, 2006). A more reliable sensitivity analysis would consider this downward trend and would be able to predict the price of ethanol and DDGS in respect of the cost of wheat and then examine the impact of the variation on the price of AX.

However, a simpler strategy was developed for the evaluation of the AX production costs in respect of the price of wheat, although the uncertainty is high. The major source of uncertainty is the assumption that the DDGS selling price is always constant at 0.1 \$/kg. The strategy also assumes that the biorefinery has always a constant economic result; a conservative annual 17% ROI. The ethanol price can now be estimated for the base case wheat-to-ethanol plant, in order for the economic target to be achieved. Similarly the AX production cost can then be estimated, such that the integrated section will contribute to the economics in proportion to the revenues (17% ROI).

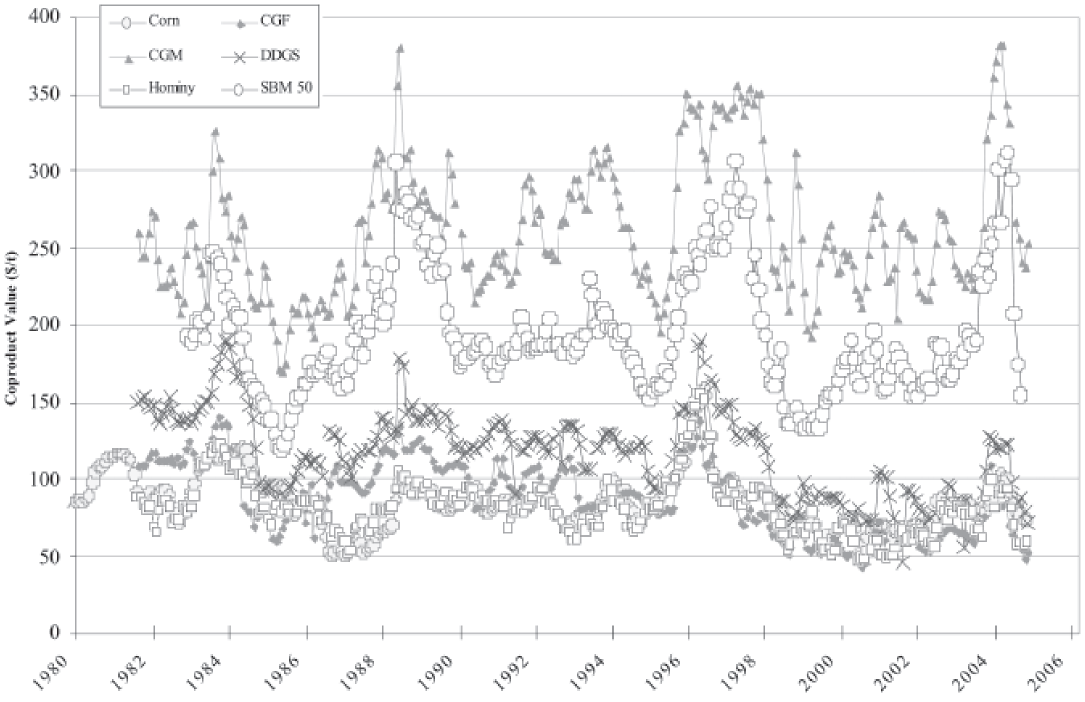


Figure 5.7. Selling prices of the corn-to-ethanol co-products (Rausch and Belyea, 2006).

Another crucial parameter for the AX co-production section is the price of hydrogen peroxide. Table 5.9 summarises the results of the sensitivity analysis. Other factors (capacity, other raw material prices) were kept constant, apart from the price of wheat or H_2O_2.

The strategy followed for AX production does not seem to be strongly dependent on the price of wheat, mainly because previously the ethanol price was fixed. The corresponding changes to the AX price are a result of the ethanol losses within the section, since they are charged to the AX. The price of hydrogen peroxide can affect the AX selling price more than the price of wheat.

Table 5.9. Sensitivity analysis in respect of the price of wheat and hydrogen peroxide. Base case: wheat price = 0.2 \$/kg, H_2O_2 price = 1.1 \$/kg, Ethanol price = 0.71 \$/kg.

	Price of variable (\$/kg)	Corresponding price of Ethanol (\$/kg)	Corresponding price of AX (\$/kg)
Wheat	0.14	0.534	7.15
Wheat	0.188	0.675	7.26
Wheat	0.2	0.71	7.3
Wheat	0.26	0.886	7.6
H_2O_2	0.7	0.71	6.6
H_2O_2	1.5	0.71	8.15

5.3 Discussion

Simulation of AX extraction in the context of a bioethanol plant indicates that the cost of producing AX would be around 7.3 \$/kg (3.65 £/kg) if AX could be recovered from bran produced by simple hammer milling, and 9.1 \$/kg (4.55 £/kg) if debranning were used to recover bran for AX extraction. These estimates are based on a bioethanol plant with a capacity of about 100 million kg per annum that utilises 4.4% of the total wheat (2 t/h) for AX co-production from the bran-rich stream, producing about 2.1 million kg per annum of an 80% purity AX product.

Other viscosity enhancers such as xanthan gum cost as much as 12 \$/kg, although others such as guar gum are much cheaper at 0.78 \$/kg (Anonymous, 1995). However it is not considered that AX rheological properties could match the unique functionality of xanthan gum (Bergmans *et al.,* 1999). Although this analysis indicates that AX could be produced at a cost comparable with other viscosity-enhancing food ingredients, it would be competing at the premium end of the market and would need to offer additional benefits such as, for example, prebiotic functionality or emulsion stability. Pharmaceutical applications may offer much higher costs, but would require further costly purification steps, and are unlikely to be able to absorb the full AX production capacity corresponding to the ethanol production of a modest plant. The current analysis draws its conclusions based on a conservative scenario of an AX ingredient intended for food use in large volumes and at modest cost.

As expected, the majority of the production costs of AX are related to the solvents. Ethanol and H_2O_2 requirements (both on a 100% basis) are 38 kg and 2 kg, respectively, for every kg of purified AX produced. The integration within a bioethanol plant effectively reduced the ethanol costs compared with those that would be incurred by a dedicated single product AX production facility. If ethanol were purchased for use within a dedicated plant producing only AX, its cost would be about 27 \$/kg of product (assuming that the ethanol would not be recycled), while its effective recycling and reuse drop the ethanol cost to about 0.92 \$/kg of AX product. Hydrogen peroxide costs represent about 30% of the total production costs, or 2.15 \$/kg of AX product.

The analogous recovery and reuse of H_2O_2 was not examined. The latter was assumed to be purchased at 1.1 \$/kg (at 100% purity) for the operation of the extraction and has a total demand of 44×10^6 kg during the 10 year life time of the plant, corresponding to over \$48 million. Integration of a recovery process would be attractive, if the additional capital investment and operating costs are less than the total costs of H_2O_2 as a purchased raw material.

Another aspect that would lower the production costs is the required level of purification. According to Hollmann and Lindhauer (2005) the product has 70% purity prior to the addition of β-glucanases. β-glucans offer both better rheological properties (Grimm *et al.*, 1995) and additional health benefits such as cholesterol lowering (Wood, 2001). It is not therefore necessary to hydrolyse them. By skipping the β-glucan degradation step, more than 1 \$/kg of product could be saved, and the product may be more functional.

Having estimated that the production cost is reasonable, the next basic step for the establishment of a market for AX in the food industry is research and development to establish opportunities for advantageous use, in particular in food products. The use in bread seems to have potential. Courtin and Delcour (2002) noted "In spite of early reports on their beneficial impact in bread-making, AX remained only a theoretical candidate for addition to the bread recipe. This is related to the fact that studies of their functionality have sometimes yielded contradictory results and to their unavailability on a commercial scale". Hollmann and Linhauer (2005) similarly comment "Whether (glucurono)arabinoxylans have any prebiotic effect is still speculative. The main reason for the relatively scarce knowledge of their nutritional impact on the human body is that these polysaccharides are still not available in quantities to perform any animal or human studies." There is a chicken and egg situation here – the potential of AX in bread (and other products) to enhance quality or as a prebiotic has not been conclusively established because of lack of a commercial source, but the commitment to produce a commercial source requires confirmation of the value of the product. Research is needed to address this impasse.

If the results of food product development are still promising, the next step would be research aimed at optimisation of the AX extraction process itself. The overall yield achieved by the extraction technique that was used was about 45-50% (Hollmann and Lindhauer, 2005), *i.e.* only half of the initial AX in the bran is finally recovered into the product. As already stated, the initial investigation of the alkaline hydrogen peroxide for AX extraction (Maes and Delcour, 2001), indicated that the yield of the polysaccharides depends on the residence time, temperature, bran solids concentration in the slurry and the hydrogen peroxide concentration. The temperature used for the extraction was 40°C (Hollmann and Lindhauer, 2005), although at 60°C the yields were significantly improved (Maes and Delcour, 2001). If the overall yield could be improved to 60% just by increasing the temperature to 60°C, then the cost of production would be reduced at least 1 \$/kg of 80% purity product. In addition if 1% H_2O_2 could be used for the extraction providing the same 50% yield (as found by Maes and Delcour, 2001), then the costs for H_2O_2 would be 50% less, and so the AX product would be \$1.07/kg cheaper. Optimisation of the extraction process could provide substantial savings.

If a food industry market could be established for AX with a selling price of around \$12/kg (£6/kg), the inclusion of AX extraction would increase the overall ROI of the plant from 17 to 26% (reducing the Payback Time to about 4 years). Alternatively, keeping the overall ROI of the biorefinery constant at 17%, the ethanol could be sold at 0.1 $/kg cheaper, giving a 14% saving on the base case price of 0.71 $/kg. This is a substantial saving which, combined with the possibility of offering a hitherto unavailable ingredient to the food industry, makes the prospect of co-producing AX with ethanol highly attractive.

Clearly there is potential to develop a market for AX as a food ingredient. The production costs indicate that this is feasible, although the estimated costs are too large to compete directly with the cheapest available viscosity-enhancing food ingredients unless AX can offer additional benefits. These additional benefits may include prebiotic functionality (Grootaert *et al*., 2007). Further research is needed to establish the prebiotic functionality of AX, to optimise the process further using better quality process data from bioethanol production specifically in the UK context, to investigate the effect of varietal, agronomic and processing factors on AX extraction and functionality, and to study practical usage of AX as an ingredient in food products.

5.4. Summary

AX co-production within a bioethanol plant was examined, according to a pilot-scale process adapted from the literature using wheat bran to produce an 80% purity AX product suitable for human consumption. The process uses large amounts of ethanol, firstly for the removal of low molecular weight contaminants, and secondly for the precipitation of the AX. This therefore allows opportunity for economic production through integration within a bioethanol plant.

The process was simulated using SuperPro Designer. Three flowsheets were developed: the base case wheat-to-ethanol plant (with structure and economic models adapted from the corn-to-ethanol process of Kwiatkowski *et al.,* 2006 and modified for wheat-to-ethanol according to Mortimer *et al.,* 2004); AX co-production by using simple hammer milling and sieving to obtain the bran-rich stream; and AX co-production using debranning to obtain bran. Both the second and third flowsheets sent 4.4% of the total wheat to the AX co-production section. The production capacity of the ethanol plant was 106 million kg ethanol per year, yielding 2.1 million kg of an 80% purity AX product.

Both ethanol and DDGS flowrates were reduced as a result of extracting AX. Ethanol was reduced by about 2.5%, due to starch and ethanol losses in the bran-rich stream and in the recycling loop, respectively, while DDGS was reduced by 8%. The AX production cost was found to be 7.3 and 9.1 $/kg (3.65 and 4.55 £/kg) without and with debranning, respectively. However, the uncertainty of the costings used for the debranning flowsheet is very high. The major contributor of the AX co-production section in both cases is the solvent used for the AX extraction, alkaline H_2O_2. The AX co-production section could be integrated into an existing wheat-to-ethanol plant.

As the price range for producing AX appears to be reasonable, further research in relation to use of AX as a food ingredient is warranted, in order to encourage a market to be established. Following establishment of a feasible market, the process could then be optimised further. It is believed that simple operating parameter changes could result in substantial reductions in the production costs, of the order of 10-20%. In addition, research into the varietal, agronomic and processing factors that affect the extraction and functionality of AX from wheat are needed to support the development of this proposed market.

Co-products are crucial to the economics of biorefineries, and therefore to the sustainability of bioethanol. The above process reduces the production of ethanol and the DDGS. Even so, if a food industry market were established for AX with a selling price of around $12/kg (£6/kg), the inclusion of AX extraction would increase the overall ROI of the plant from 17 to 26%. Alternatively, keeping the overall ROI of the biorefinery constant at 17%, the ethanol could be sold at 0.1 $/kg cheaper, giving a 14% saving on the base case price of 0.71 $/kg. This is a substantial saving which, combined with the possibility of offering a hitherto unavailable ingredient to the food industry, makes the prospect of co-producing AX with ethanol highly attractive. It argues for substantial research in this area to bring about this development and thereby to facilitate the introduction of bioethanol production in the UK, leading to the establishment of wheat biorefineries more generally.

6. Conclusions and Recommendations

6.1. Progress made in the current work

Bioethanol production in the UK requires the production of co-products in order to allow viable commercial operation to be achieved at an early stage. At the same time, the interesting potential of arabinoxylans in several food and non-food applications cannot currently be realised, due to lack of a commercial source. There is an opportunity to address these two issues together by integrating AX extraction from bran with bioethanol production from wheat in an integrated biorefinery. This has the potential to enhance the economics of ethanol production while making an AX product commercially available, provided AX extraction can be implemented cost-effectively. The current work therefore evaluated the likely production costs of AX if co-produced in a biorefinery principally producing bioethanol. The work also investigated the potential for employing pearling (debranning) technology within bioethanol production. By compiling relevant data and exploring the conceptual and practical issues, the work has also established and demonstrated the framework by which the potential of other co-products beyond AX (such as succinic acid) might be evaluated.

The major conclusions of the work are as follows:

- Using debranning to remove a portion of the bran to bypass the ethanol production process (to reduce drying costs and water usage in the process) is not economical, because the additional electricity costs of debranning, the reduced ethanol yield due to starch losses, and the capital cost of the debranner, outweigh the savings in drying costs.
- Debranning would only be of benefit in a wheat bioethanol plant as a convenient way of recovering bran for further processing, *e.g.* for extraction of high value products from the bran.
- Arabinoxylans are a promising co-product for extraction from wheat bran, being present in wheat bran at high concentrations, and with several interesting functional properties including viscosity enhancement, emulsion or foam stabilisation, water absorption, thickening, gelling, fat replacement, a source for the production of oligosaccharides, and possible physiological (prebiotic) benefits.
- Based on literature reports, AX suitable for food use can be extracted from wheat bran using alkaline hydrogen peroxide, with ethanol used for bran washing and AX precipitation, and the extract purified with enzymatic treatments.
- Bran for AX extraction could be obtained by debranning, by roller milling and sifting, or by hammer milling. Alternatively bran could be purchased from an external source, *e.g.* from a flour miller.
- AX concentration appears to be higher in the outer bran layers than in the rest of the bran. Recovery of bran via debranning may yield a bran source that is enriched in AX, facilitating economic extraction of the AX. However, the fine bran may give problems with dewatering and handling. The practicalities of handling the fine bran powder produced by debranning

need to be investigated. Also, the functionality of AX extracted from bran from different parts of the wheat kernel, and from a wide range of wheats, needs to be investigated.

- Starch in bran could be recovered for ethanol production by washing the bran with water prior to extraction, and sending the water plus starch to the liquefaction stage. Simple water washing allowed recovery of 70-75% of the starch in the bran.
- Value Analysis is a powerful tool for optimising process networks and identifying unprofitable streams, which with more information from actual plants could be adapted to enhance the operation of cereal biorefineries.
- After wheat, the major raw materials costs for ethanol production are the enzymes, while the major raw materials cost for AX extraction is the hydrogen peroxide.
- After raw materials, utilities comprise the next major operating cost, with steam making the largest contribution. The addition of AX extraction increases steam usage due to the additional distillation requirement of the recycled ethanol.
- Based on simulations using SuperPro Designer of a plant producing around 100 million kg per annum of ethanol and 2.1 million kg per annum of AX, it was estimated that an AX product of 80% purity could be co-produced with ethanol and DDGS at a cost of around £3.6-4.6 per kg.
- AX production using hammer milling of the wheat and recovery of bran via sieving appeared to be cheaper than using debranning to obtain the bran. However, the higher concentration of bran in the outer layers of wheat, *i.e.* those selectively recovered by debranning, could offset the additional costs of debranning by facilitating extraction, provided the AX extracted from these outer layers exhibits good functional properties.
- The estimated costs for AX production are within the range of comparable viscosity-enhancing ingredients used in the food industry, but are towards the top end of the range. In order to establish a market for such a product, it would need to offer additional benefits such as, for example, prebiotic functionality or emulsion stability.
- Optimisation of the AX extraction process could reduce the costs of AX production by around 10-20%.
- Retaining the β-glucan, rather than adding enzymes to degrade it in order to enhance AX content in the final product, could provide a more valuable and functional product and further reduce production costs by around 10-15%.
- If a food industry market could be established for AX with a selling price of around £6/kg, the inclusion of AX extraction would increase the overall ROI of the plant from 17 to 26% (reducing the Payback Time to about 4 years). Alternatively, keeping the overall ROI of the biorefinery constant at 17%, the ethanol could be sold at a price 14% less than for the base case of conventional ethanol production.

- A pharmaceutical AX product could have a much higher value; however, the size of the market is likely to be smaller than for an AX-based food ingredient, and additional costly purification steps would be required. In the first instance, aiming to establish a food market for AX is probably safer.
- The estimated costs for producing AX in the context of bioethanol production are sufficiently attractive that further research on the functionality of wheat-derived AX and its practical use for food and/or pharmaceutical applications is warranted.

6.2. Recommendations for future work

Production of ethanol from wheat in the UK would give several benefits: alleviation of the production of greenhouse gases contributing to global warming; increased national fuel security; and enhanced national agriculture and rural life. In particular, wheat growers would see their crop increased in value and serving a larger and more diverse market with a greater range of valuable end products. The need to produce fuel ethanol economically, and the opportunity to create a valuable new wheat-derived product, together make the prospect of co-production of ethanol and AX highly desirable. The current work has indicated that the production costs of AX are sufficiently low to be commercially feasible, but that AX could only compete and create a market as a food ingredient if it offered additional benefits beyond viscosity enhancement. Research to establish those benefits and to enhance AX extraction through process optimisation and through identification of the most suitable wheat varieties and agronomic practices for AX yield and functionality is therefore justified and should be pursued.

Critical questions surround (i) the sourcing and functionality of AX; (ii) process optimisation; and (iii) applications of AX for food and non-food uses.

Bran for AX extraction could be obtained from the outer layers of the wheat kernel (via debranning), or from the inner layers and crease bran (by milling pearled wheat), or from the entire unfractionated bran component of the wheat. Evidence presented in the current work suggests that the outer layers may be enriched in AX and that bran recovered by debranning may therefore offer advantages. However the yield and functionality of the AX so obtained, compared with that from other parts of the kernel, need to be investigated comprehensively.

Beyond this, it is highly probably that different wheat varieties yield bran more or less suited to AX extraction, and that the AX extracted varies in its functional properties. Similarly, it is likely that agronomic practices and environmental conditions during growing of the crop affect AX. Effective co-production of AX with bioethanol will require detailed understanding of the factors affecting the inherent quality of AX in wheat.

There appears to be significant scope for optimising the AX extraction process, in particular to reduce hydrogen peroxide usage through extraction at lower H_2O_2 concentrations and through recovery and recycling of the H_2O_2. The practicalities of processing bran, particularly fine bran powder, also need to be investigated in order to be able to design industrial scale AX extraction processes with confidence.

Finally, it is clear that AX offers several applications in both the food and the non-food areas. However, not all of the potential applications of AX have been established for wheat-derived AX, and not all of the suggested benefits have been demonstrated in practice. For example, the use of wheat AX in bread and baked products appears promising, but the necessary research has been precluded for lack of a commercial source of AX. Similarly the suggestion of prebiotic activity of AX needs to be confirmed and investigated more thoroughly. Research into practical usage of AX in various food products and for non-food applications needs to be undertaken, to establish the potential to create a market for this novel but untested product.

The opportunities to facilitate the introduction of fuel ethanol production into the UK, to decrease the cost of fuel ethanol, to ensure that the UK bioethanol uses wheat as its feedstock of choice, and to create a commercial source of a valuable new product together offer significant benefits to UK society and to the primary producers of wheat. The current work has confirmed that pursuing AX production from wheat within the context of the incipient UK bioethanol industry is justifiable and worthy of continued research activity and support.

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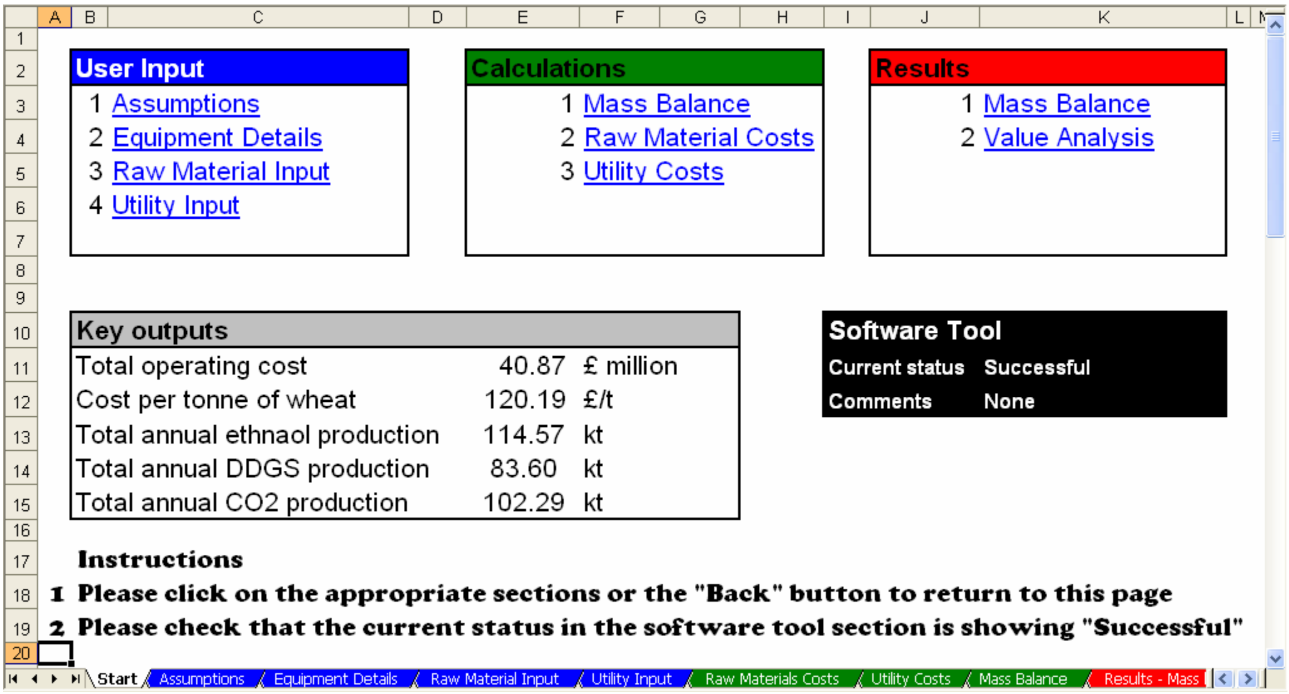
Appendices

Appendix A
Software Tool

Start
This is the initial starting point for any user of the tool. The worksheet contains five sections. The three top sections (Figure A1) provide an easy way of navigating the tool through simply clicking the required option. Each worksheet also contains a "back" arrow shaped button to return to the "Start" worksheet. The other section shown to the lower left of Figure A1 shows the key outputs for the model. For more detailed results the user is requested to proceed to the Results section.

Finally, to the right bottom of Figure A1 there is a software tool section for error handling. The user needs to pay special attention to the current status of the model and make sure that it is showing "Successful"; otherwise the user needs to check the wheat/bran composition.



User Input
1 Assumptions
2 Equipment Details
3 Raw Material Input
4 Utility Input

Calculations
1 Mass Balance
2 Raw Material Costs
3 Utility Costs

Results
1 Mass Balance
2 Value Analysis

Key outputs		
Total operating cost	40.87	£ million
Cost per tonne of wheat	120.19	£/t
Total annual ethnaol production	114.57	kt
Total annual DDGS production	83.60	kt
Total annual CO2 production	102.29	kt

Software Tool
Current status Successful
Comments None

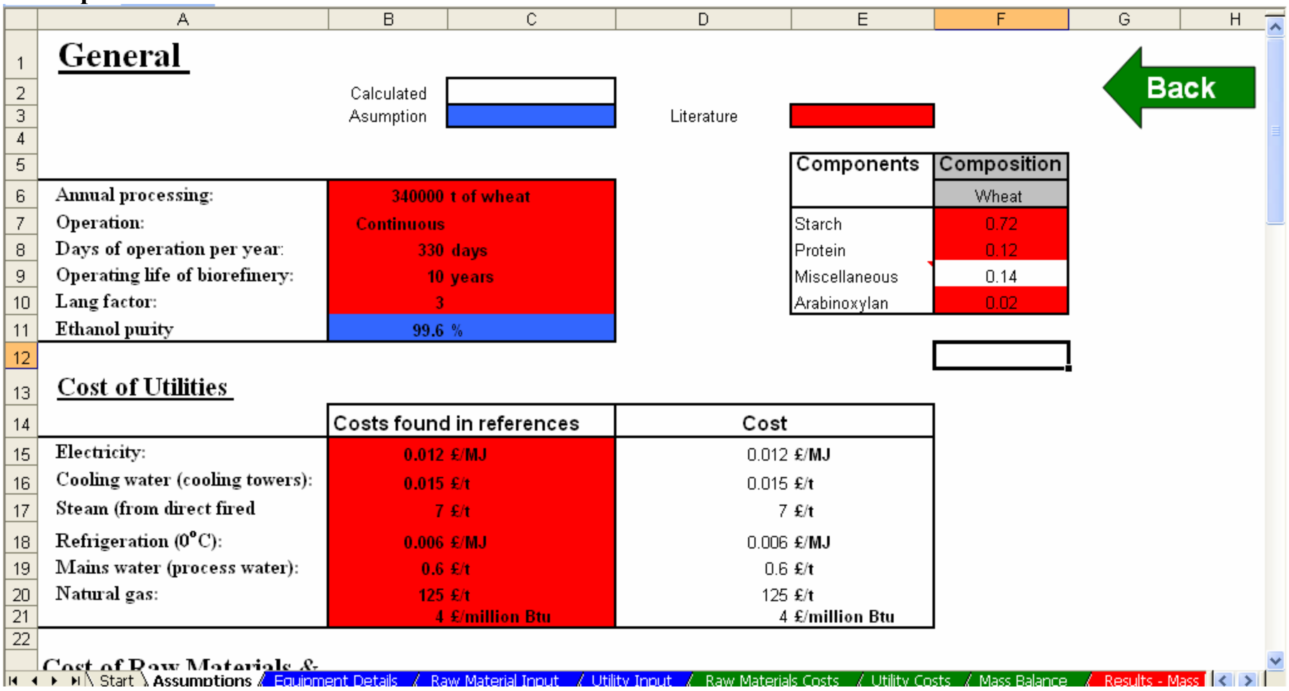
Instructions
1 Please click on the appropriate sections or the "Back" button to return to this page
2 Please check that the current status in the software tool section is showing "Successful"

Figure A1. Start – Main starting point for any simulation.

User Input
The following 4 sections could be modified by the user:

- Assumptions
- Equipment Detail
- Raw material Input
- Utility Input

Assumptions



General

Calculated ☐
Asumption 🟦
Literature 🟥

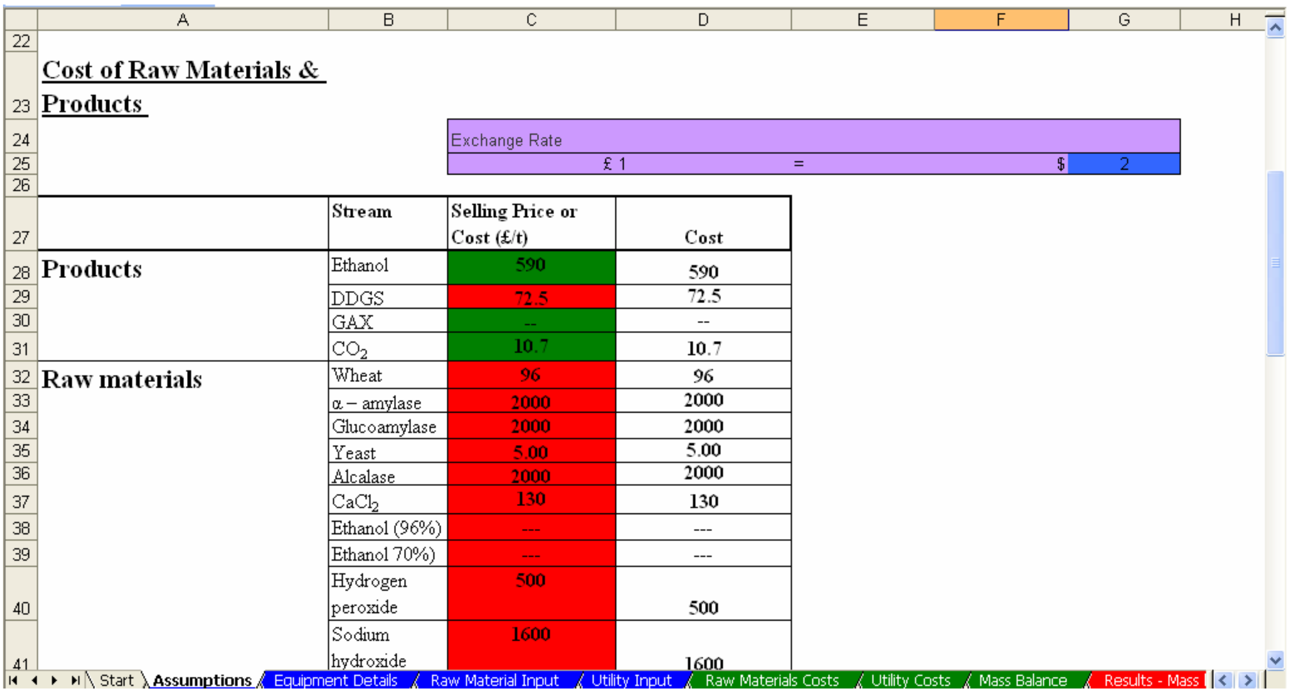
Annual processing:	340000 t of wheat
Operation:	Continuous
Days of operation per year:	330 days
Operating life of biorefinery:	10 years
Lang factor:	3
Ethanol purity	99.6 %

Components	Composition
	Wheat
Starch	0.72
Protein	0.12
Miscellaneous	0.14
Arabinoxylan	0.02

Cost of Utilities

	Costs found in references	Cost
Electricity:	0.012 £/MJ	0.012 £/MJ
Cooling water (cooling towers):	0.015 £/t	0.015 £/t
Steam (from direct fired	7 £/t	7 £/t
Refrigeration (0°C):	0.006 £/MJ	0.006 £/MJ
Mains water (process water):	0.6 £/t	0.6 £/t
Natural gas:	125 £/t 4 £/million Btu	125 £/t 4 £/million Btu

Figure A2. Assumptions section showing where the user can change various assumptions (e.g. wheat/bran composition and the price of the various raw materials and products).



Cost of Raw Materials & Products

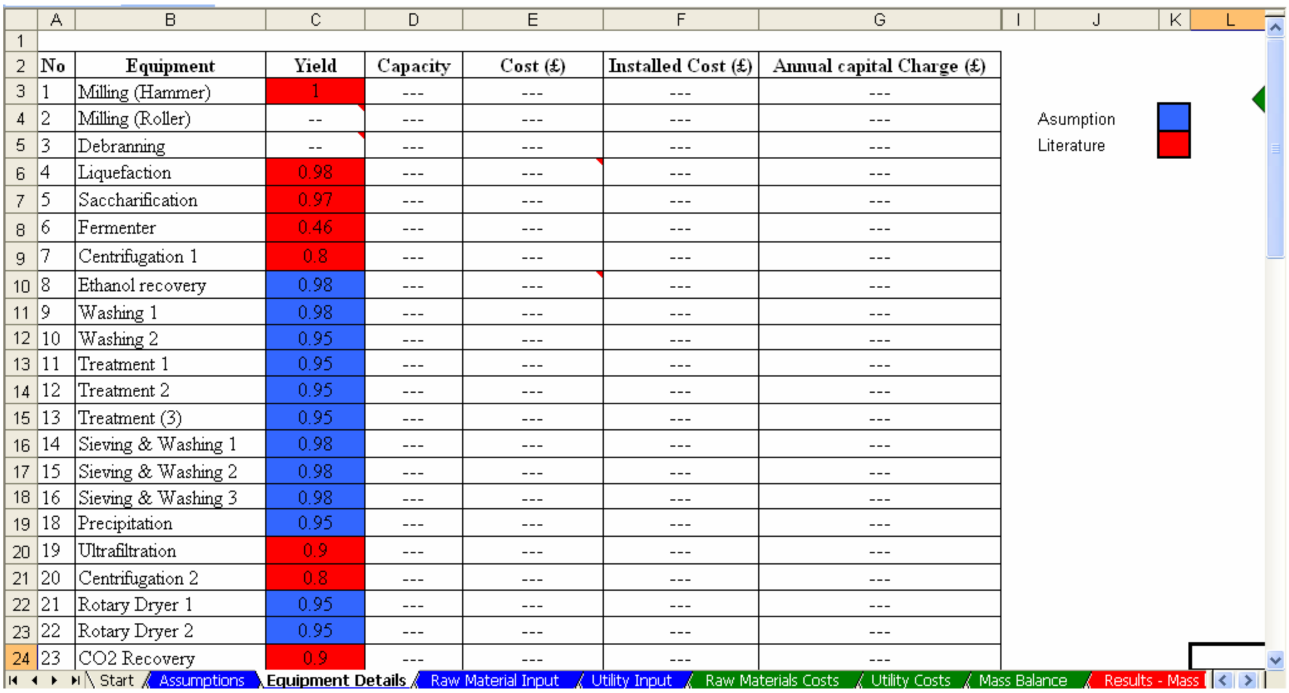
Exchange Rate
£ 1 = $ 2

	Stream	Selling Price or Cost (£/t)	Cost
Products	Ethanol	590	590
	DDGS	72.5	72.5
	GAX	--	--
	CO_2	10.7	10.7
Raw materials	Wheat	96	96
	α – amylase	2000	2000
	Glucoamylase	2000	2000
	Yeast	5.00	5.00
	Alcalase	2000	2000
	$CaCl_2$	130	130
	Ethanol (96%)	---	---
	Ethanol 70%)	---	---
	Hydrogen peroxide	500	500
	Sodium hydroxide	1600	1600

Figure A2 continued

Equipment Detail

This section allows the user to specify the step yield of the various unit operations. The equipment cost could also be added in the future.

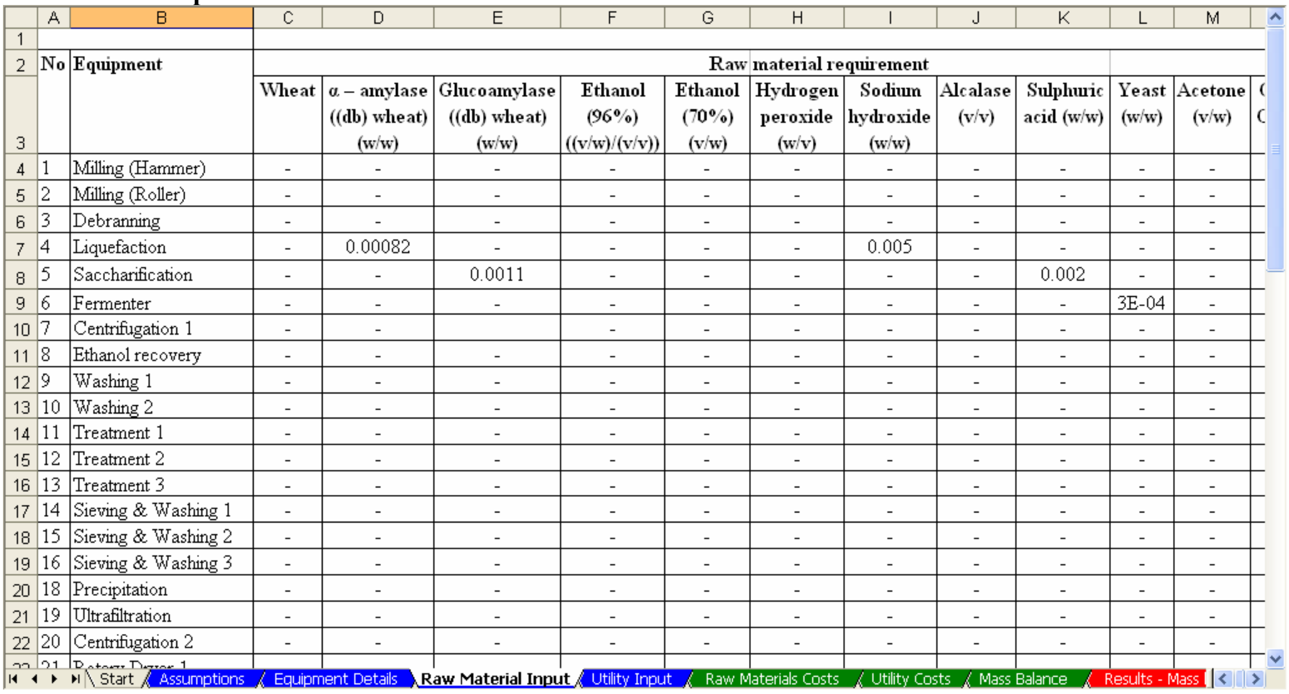


No	Equipment	Yield	Capacity	Cost (£)	Installed Cost (£)	Annual capital Charge (£)
1	Milling (Hammer)	1	---	---	---	---
2	Milling (Roller)	--	---	---	---	---
3	Debranning	--	---	---	---	---
4	Liquefaction	0.98	---	---	---	---
5	Saccharification	0.97	---	---	---	---
6	Fermenter	0.46	---	---	---	---
7	Centrifugation 1	0.8	---	---	---	---
8	Ethanol recovery	0.98	---	---	---	---
9	Washing 1	0.98	---	---	---	---
10	Washing 2	0.95	---	---	---	---
11	Treatment 1	0.95	---	---	---	---
12	Treatment 2	0.95	---	---	---	---
13	Treatment (3)	0.95	---	---	---	---
14	Sieving & Washing 1	0.98	---	---	---	---
15	Sieving & Washing 2	0.98	---	---	---	---
16	Sieving & Washing 3	0.98	---	---	---	---
18	Precipitation	0.95	---	---	---	---
19	Ultrafiltration	0.9	---	---	---	---
20	Centrifugation 2	0.8	---	---	---	---
21	Rotary Dryer 1	0.95	---	---	---	---
22	Rotary Dryer 2	0.95	---	---	---	---
23	CO2 Recovery	0.9	---	---	---	---

Asumption 🟦
Literature 🟥

Figure A3. Equipment detail section where the user can specify equipment step yield.

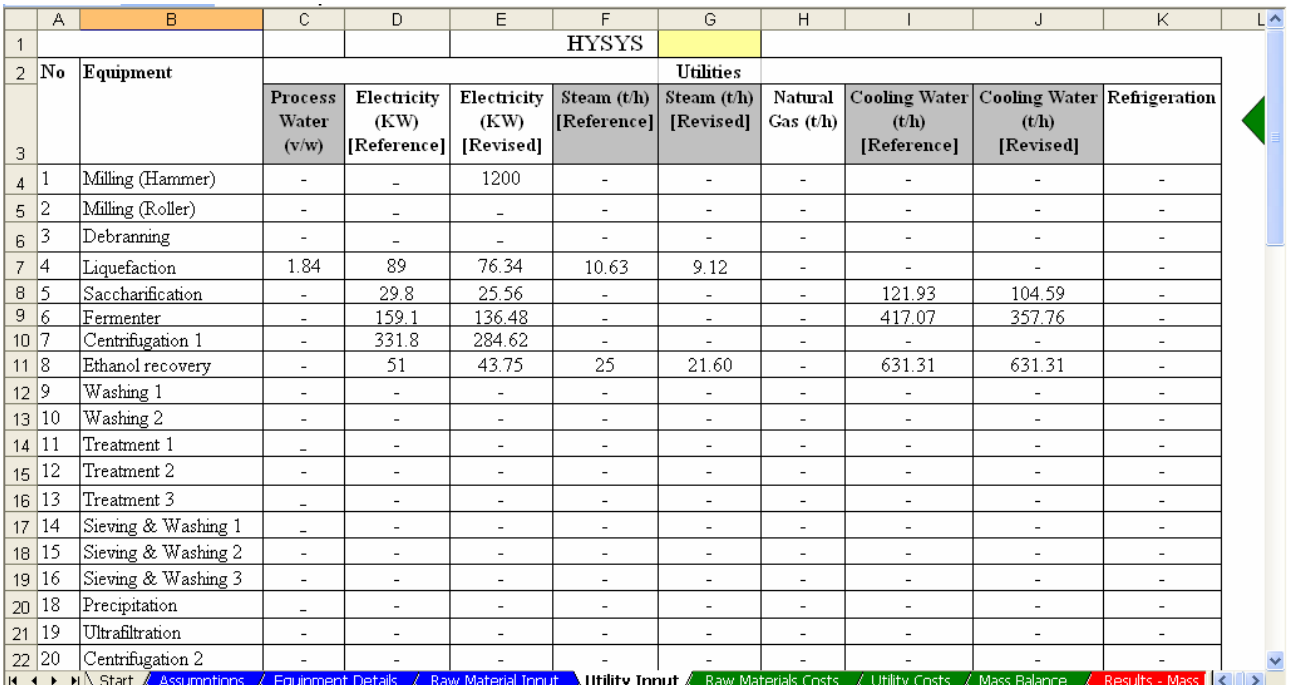
Raw Material Input



No	Equipment	Raw material requirement										
		Wheat	α – amylase ((db) wheat) (w/w)	Glucoamylase ((db) wheat) (w/w)	Ethanol (96%) ((v/w)/(v/v))	Ethanol (70%) (v/w)	Hydrogen peroxide (w/v)	Sodium hydroxide (w/w)	Alcalase (v/v)	Sulphuric acid (w/w)	Yeast (w/w)	Acetone (v/w)
1	Milling (Hammer)	-	-	-	-	-	-	-	-	-	-	-
2	Milling (Roller)	-	-	-	-	-	-	-	-	-	-	-
3	Debranning	-	-	-	-	-	-	-	-	-	-	-
4	Liquefaction	-	0.00082	-	-	-	-	0.005	-	-	-	-
5	Saccharification	-	-	0.0011	-	-	-	-	-	0.002	-	-
6	Fermenter	-	-	-	-	-	-	-	-	-	3E-04	-
7	Centrifugation 1	-	-		-	-	-	-	-	-	-	-
8	Ethanol recovery	-	-	-	-	-	-	-	-	-	-	-
9	Washing 1	-	-	-	-	-	-	-	-	-	-	-
10	Washing 2	-	-	-	-	-	-	-	-	-	-	-
11	Treatment 1	-	-	-	-	-	-	-	-	-	-	-
12	Treatment 2	-	-	-	-	-	-	-	-	-	-	-
13	Treatment 3	-	-	-	-	-	-	-	-	-	-	-
14	Sieving & Washing 1	-	-	-	-	-	-	-	-	-	-	-
15	Sieving & Washing 2	-	-	-	-	-	-	-	-	-	-	-
16	Sieving & Washing 3	-	-	-	-	-	-	-	-	-	-	-
18	Precipitation	-	-	-	-	-	-	-	-	-	-	-
19	Ultrafiltration	-	-	-	-	-	-	-	-	-	-	-
20	Centrifugation 2	-	-	-	-	-	-	-	-	-	-	-
21	Rotary Dryer 1											

Figure A4. Raw material input section where the user can specify the loadings for the various raw materials.

Utility Input

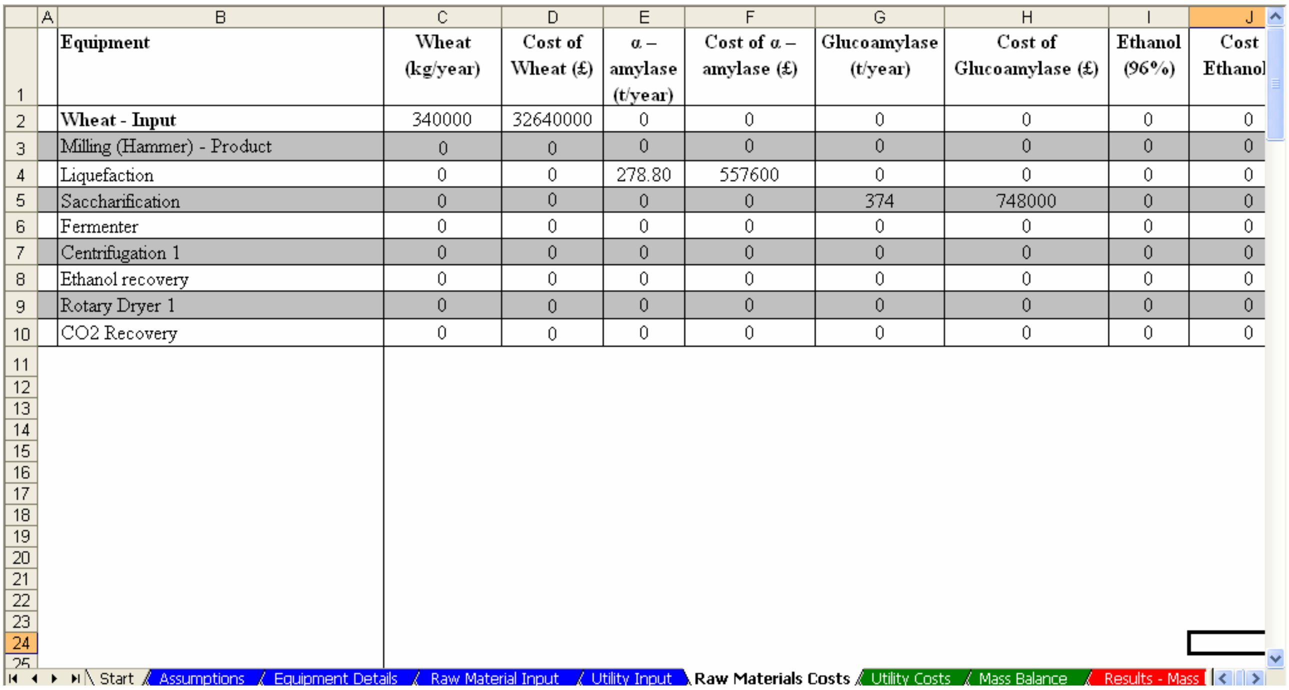


		HYSYS								
No	Equipment					Utilities				
		Process Water (v/w)	Electricity (KW) [Reference]	Electricity (KW) [Revised]	Steam (t/h) [Reference]	Steam (t/h) [Revised]	Natural Gas (t/h)	Cooling Water (t/h) [Reference]	Cooling Water (t/h) [Revised]	Refrigeration
1	Milling (Hammer)	-	-	1200	-	-	-	-	-	-
2	Milling (Roller)	-	-	-	-	-	-	-	-	-
3	Debranning	-	-	-	-	-	-	-	-	-
4	Liquefaction	1.84	89	76.34	10.63	9.12	-	-	-	-
5	Saccharification	-	29.8	25.56	-	-	-	121.93	104.59	-
6	Fermenter	-	159.1	136.48	-	-	-	417.07	357.76	-
7	Centrifugation 1	-	331.8	284.62	-	-	-	-	-	-
8	Ethanol recovery	-	51	43.75	25	21.60	-	631.31	631.31	-
9	Washing 1	-	-	-	-	-	-	-	-	-
10	Washing 2	-	-	-	-	-	-	-	-	-
11	Treatment 1	-	-	-	-	-	-	-	-	-
12	Treatment 2	-	-	-	-	-	-	-	-	-
13	Treatment 3	-	-	-	-	-	-	-	-	-
14	Sieving & Washing 1	-	-	-	-	-	-	-	-	-
15	Sieving & Washing 2	-	-	-	-	-	-	-	-	-
16	Sieving & Washing 3	-	-	-	-	-	-	-	-	-
18	Precipitation	-	-	-	-	-	-	-	-	-
19	Ultrafiltration	-	-	-	-	-	-	-	-	-
20	Centrifugation 2	-	-	-	-	-	-	-	-	-

Figure A5. Utility input section. The column termed "Revised" should not be changed as the model scale up/down according to flowrate as computed in the mass balance section.

Calculations

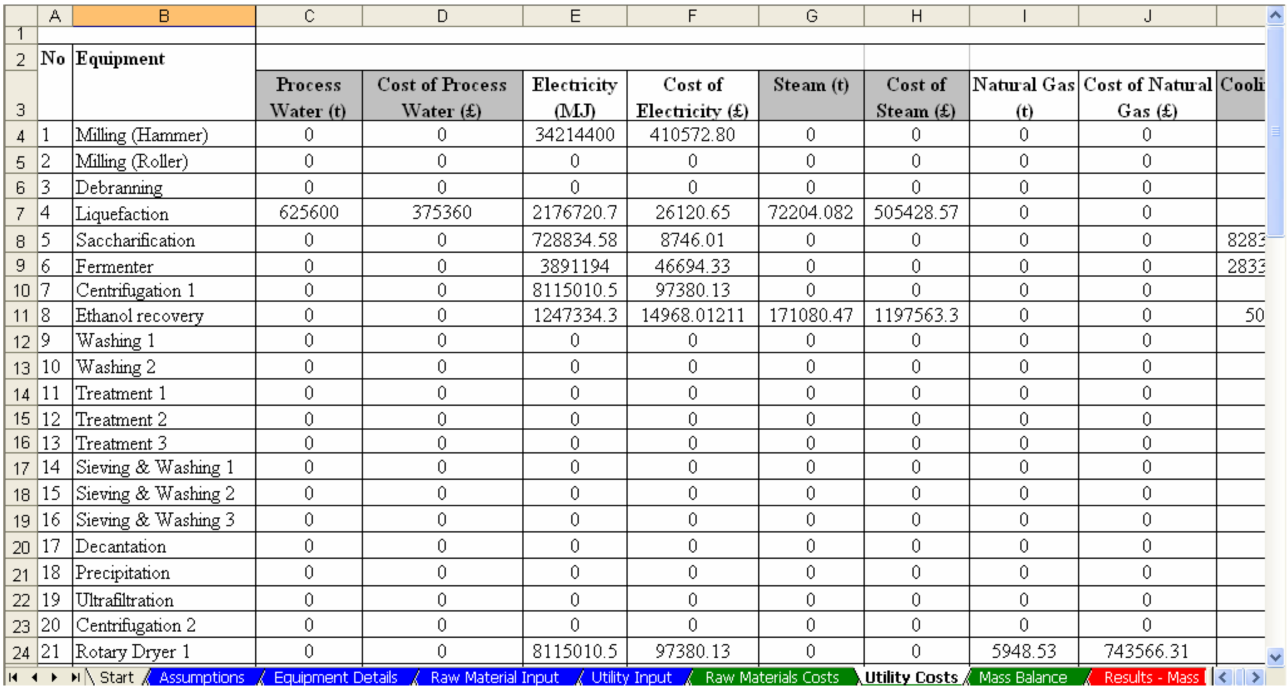
Raw Material Costs



Equipment	Wheat (kg/year)	Cost of Wheat (£)	α – amylase (t/year)	Cost of α – amylase (£)	Glucoamylase (t/year)	Cost of Glucoamylase (£)	Ethanol (96%)	Cost Ethanol
Wheat - Input	340000	32640000	0	0	0	0	0	0
Milling (Hammer) - Product	0	0	0	0	0	0	0	0
Liquefaction	0	0	278.80	557600	0	0	0	0
Saccharification	0	0	0	0	374	748000	0	0
Fermenter	0	0	0	0	0	0	0	0
Centrifugation 1	0	0	0	0	0	0	0	0
Ethanol recovery	0	0	0	0	0	0	0	0
Rotary Dryer 1	0	0	0	0	0	0	0	0
CO2 Recovery	0	0	0	0	0	0	0	0

Figure A6. The following section calculates the raw material costs.

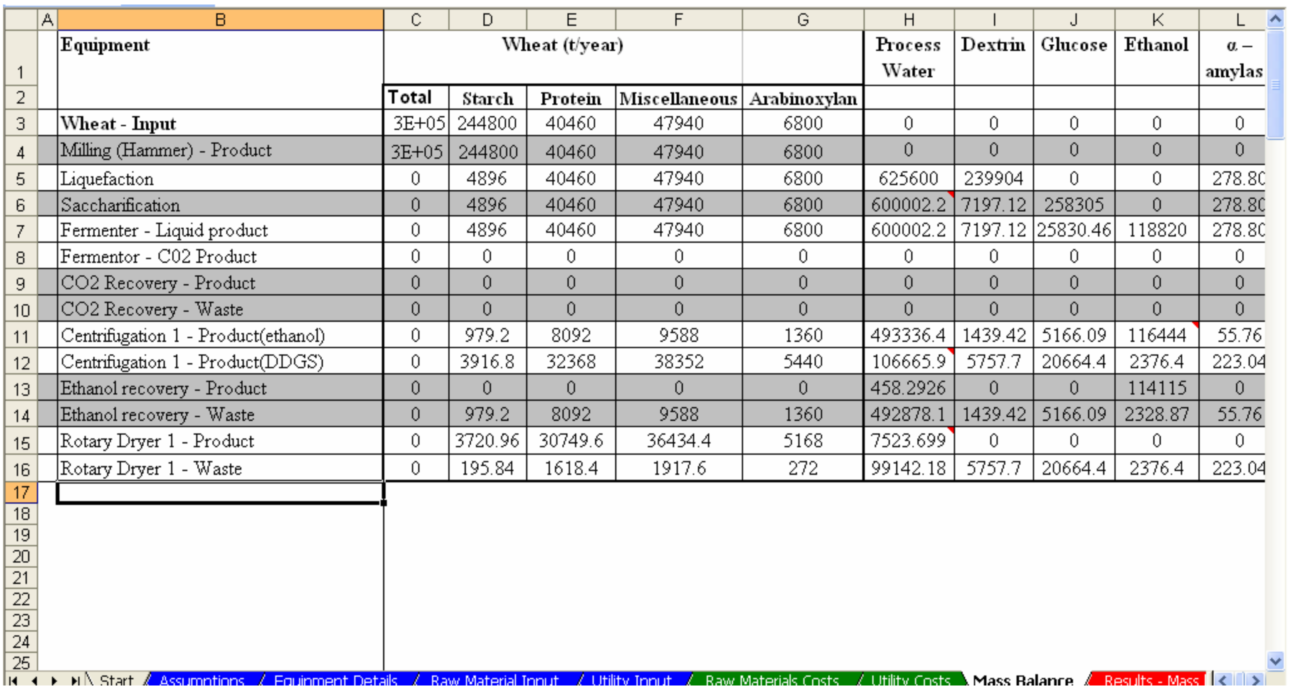
Utility Costs



No	Equipment	Process Water (t)	Cost of Process Water (£)	Electricity (MJ)	Cost of Electricity (£)	Steam (t)	Cost of Steam (£)	Natural Gas (t)	Cost of Natural Gas (£)	Cooli
1	Milling (Hammer)	0	0	34214400	410572.80	0	0	0	0	
2	Milling (Roller)	0	0	0	0	0	0	0	0	
3	Debranning	0	0	0	0	0	0	0	0	
4	Liquefaction	625600	375360	2176720.7	26120.65	72204.082	505428.57	0	0	
5	Saccharification	0	0	728834.58	8746.01	0	0	0	0	8283
6	Fermenter	0	0	3891194	46694.33	0	0	0	0	2833
7	Centrifugation 1	0	0	8115010.5	97380.13	0	0	0	0	
8	Ethanol recovery	0	0	1247334.3	14968.01211	171080.47	1197563.3	0	0	50
9	Washing 1	0	0	0	0	0	0	0	0	
10	Washing 2	0	0	0	0	0	0	0	0	
11	Treatment 1	0	0	0	0	0	0	0	0	
12	Treatment 2	0	0	0	0	0	0	0	0	
13	Treatment 3	0	0	0	0	0	0	0	0	
14	Sieving & Washing 1	0	0	0	0	0	0	0	0	
15	Sieving & Washing 2	0	0	0	0	0	0	0	0	
16	Sieving & Washing 3	0	0	0	0	0	0	0	0	
17	Decantation	0	0	0	0	0	0	0	0	
18	Precipitation	0	0	0	0	0	0	0	0	
19	Ultrafiltration	0	0	0	0	0	0	0	0	
20	Centrifugation 2	0	0	0	0	0	0	0	0	
21	Rotary Dryer 1	0	0	8115010.5	97380.13	0	0	5948.53	743566.31	

A8: The following section calculates the utility costs

Mass Balance

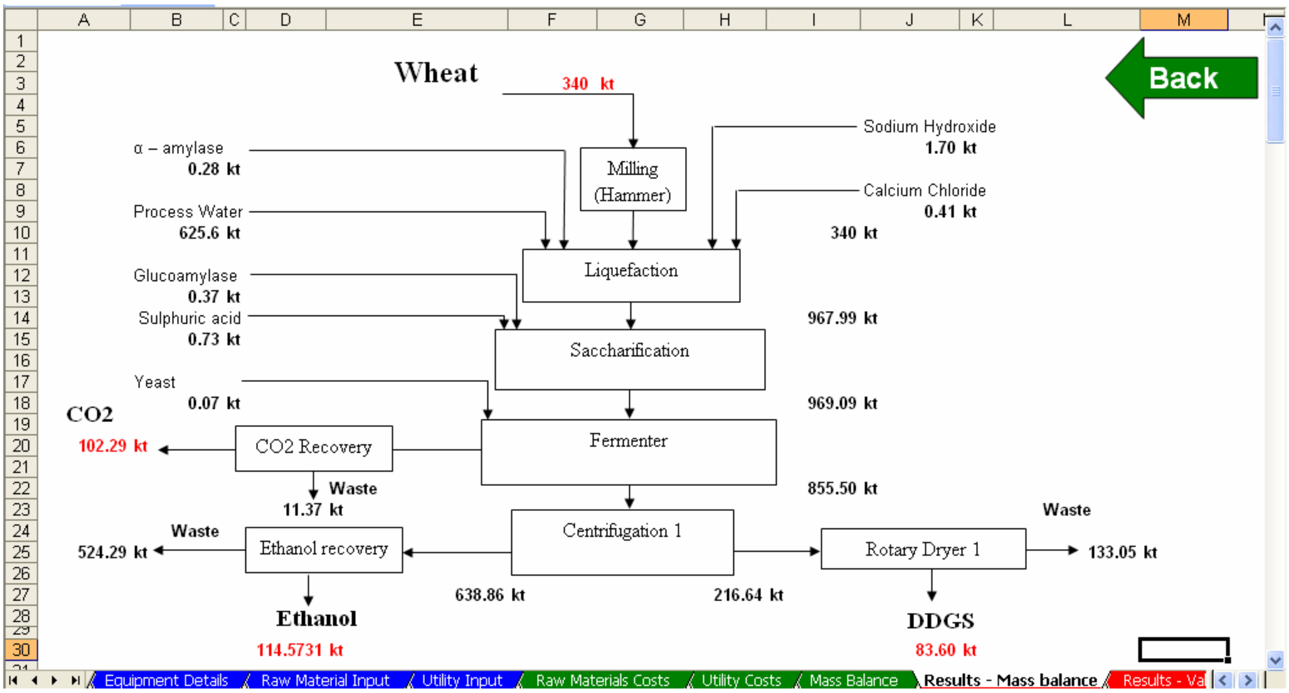


Equipment	Wheat (t/year)					Process Water	Dextrin	Glucose	Ethanol	α – amylas
	Total	Starch	Protein	Miscellaneous	Arabinoxylan					
Wheat - Input	3E+05	244800	40460	47940	6800	0	0	0	0	0
Milling (Hammer) - Product	3E+05	244800	40460	47940	6800	0	0	0	0	0
Liquefaction	0	4896	40460	47940	6800	625600	239904	0	0	278.80
Saccharification	0	4896	40460	47940	6800	600002.2	7197.12	258305	0	278.80
Fermenter - Liquid product	0	4896	40460	47940	6800	600002.2	7197.12	25830.46	118820	278.80
Fermentor - C02 Product	0	0	0	0	0	0	0	0	0	0
CO2 Recovery - Product	0	0	0	0	0	0	0	0	0	0
CO2 Recovery - Waste	0	0	0	0	0	0	0	0	0	0
Centrifugation 1 - Product(ethanol)	0	979.2	8092	9588	1360	493336.4	1439.42	5166.09	116444	55.76
Centrifugation 1 - Product(DDGS)	0	3916.8	32368	38352	5440	106665.9	5757.7	20664.4	2376.4	223.04
Ethanol recovery - Product	0	0	0	0	0	458.2926	0	0	114115	0
Ethanol recovery - Waste	0	979.2	8092	9588	1360	492878.1	1439.42	5166.09	2328.87	55.76
Rotary Dryer 1 - Product	0	3720.96	30749.6	36434.4	5168	7523.699	0	0	0	0
Rotary Dryer 1 - Waste	0	195.84	1618.4	1917.6	272	99142.18	5757.7	20664.4	2376.4	223.04

Figure A7. This section contains the mass balance calculations for the model. This makes up the main engine behind the tool.

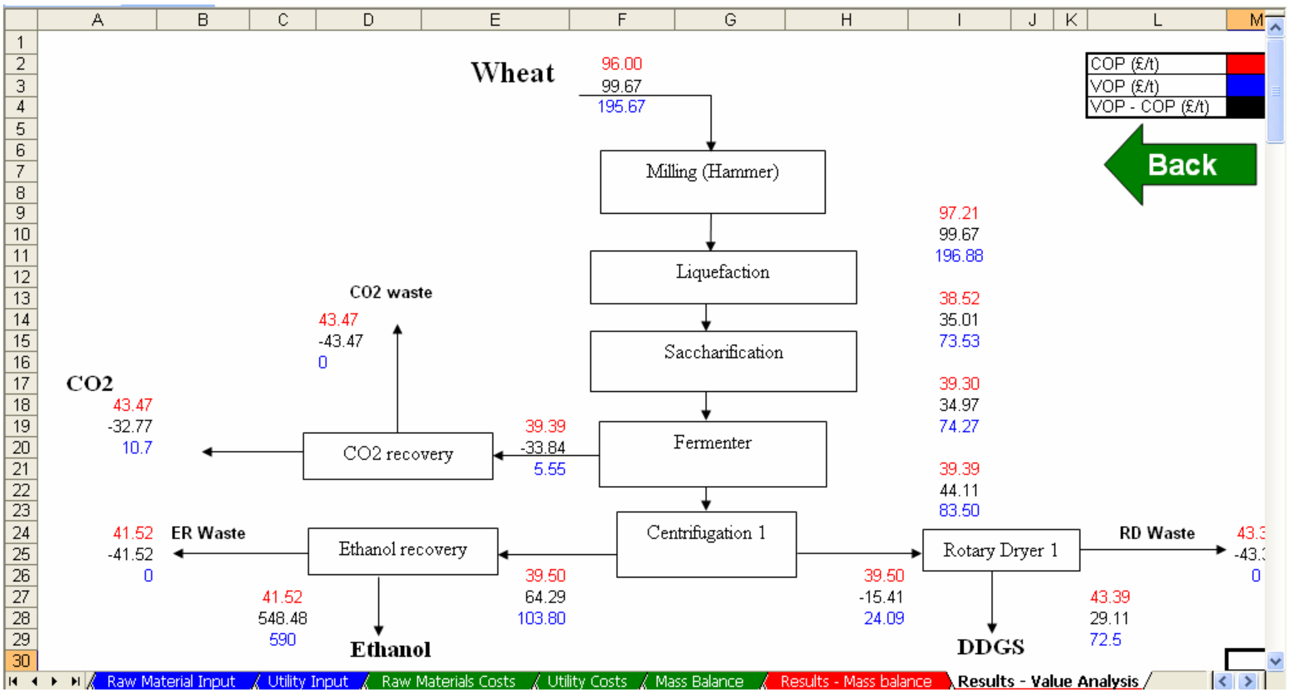
Outputs

Results - Mass balance



A10: Mass balance results section

Results - Value analysis



A11: Value analysis output results. For every stream the top value is the *Cost of Production*, the middle value is the economic margin, and the lower value is the *Value on Processing*

Appendix B
Biorefinery – Data Sheet

General Assumptions

Annual processing of 340, 000 tonnes of wheat
Operation: Continuous
Days of operation per year: 330 days

Wheat composition [a]

Composition	Composition (% dry basis)
Starch	69
Sugar	3
Protein	11.5
Non-starch polysaccharides	11
Lipid	2.5
Ash	2
Lignin	1

Cost of Utilities

Electricity: 0.012£/MJ [b]
Cooling water (cooling towers): 0.015£/t [b]
Steam (from direct fired boilers): 7£/t [b]
Refrigeration (0°C): 0.006£/MJ [b]
Mains water (process water): 0.6£/t [b]
Natural gas: 4£/million Btu [b] (125£/t)

Raw Materials & Products

Stream		Price
Products	Ethanol	£590/t [c]
	DDGS	£65-80/t [d]
	CO_2	£10.7/t [c]
	All waste stream	0
Raw materials	Wheat	£96/t [c]
	α – amylase	£2000/t [e]
	Glucoamylase	£2000/t [e]
	Yeast	£6.67/t [e]
	Alcalase	£2000/t (assume similar to other enzymes)
	β-glucosidase	£2000/t (assume similar to other enzymes)
	Lichenase	£2000/t (assume similar to other enzymes)
	$CaCl_2$	£130/t [b]
	Hydrogen peroxide (2%)	£500/t [b]
	Sodium hydroxide (25%)	£1600/t [b]
	Conc. Sulphuric acid	£40/t [b]

Equipment (1)

Equipment	Yield
Milling (Hammer)	100%
Milling (Roller)	Bran = 12-16% of wheat
Debranning	Bran = 4-8% of wheat
Liquefaction	98 % yield weight (Starch to dextrin) [g]
Saccharification	97 % yield weight (Dextrin to sugars) [g]
Fermenter	46 % yield weight (Utilizable sugars to ethanol) [g]
Centrifugation	80 % [h]
Ethanol recovery	98% (assumed)
Washing 1	98% (assumed)
Washing 2	95% (assumed)
All treatment steps	95% (assumed)
All Sieving & Washing	98% (assumed)
Precipitation	95% (assumed)
Ultrafiltration	90% (assumed)
Rotary Dryer	95% (assumed)
CO2 Recovery	90% (assumed)

Raw Material Requirements (1)

Equipment	Raw material requirement			
	α – amylase	**Glucoamylase**	**Ethanol (96%)**	**Ethanol (70%)**
Liquefaction	0.082% (db) corn [i] (assume similar to wheat)	-	-	-
Saccharification	-	0.11% (db) corn [i] (assume similar to wheat)	-	-
Washing 2	-	-	300% (assumed)	-
Treatment 1	-	-	-	600% [j]
Sieving & Washing 1	-	-	-	300% (assumed)
Precipitation	-	-	Add up to a final conc. of 65% [j]	-

Raw Material Requirements (2)

Equipment	Raw material requirement			
	Hydrogen peroxide	**Sodium hydroxide**	**Alcalase**	**Sulphuric acid**
Liquefaction	-	0.5% kg/kg corn [k] (assume similar to wheat)	-	-
Saccharification	-	-	-	0.2 % kg/kg corn [k] (assume similar to wheat)
Treatment 3	40% [j]	0.5 % (assume similar to Liquefaction)	0.125% (v/v) to reactor contents [j]	0.2% kg/kg corn (assume similar to Saccharification)

Raw Material Requirements (3)

Equipment	Raw material requirement			
	Yeast	**B-glucosidase**	**Lichenase**	**Calcium Chloride**
Liquefaction	-	-	-	0.12% (w/w) lime/corn (assume similar on a wheat basis) [g]
Fermenter	0.026%, w/w (yeast/corn) [i] (assume similar to wheat)	-	-	-
Treatment 4	-	0.125% (similar to Alcalase)	0.125% (similar to Alcalase)	-

Utility Requirements (1)

Equipment	Utilities		
	Process water	**Electricity**	**Steam**
Milling (Hammer)	-	1200KW [l] (However, if a hammer milling operation is preceded by debranning, the utility consumption = 1000KW [l])	-
Milling (Roller)	-	1250KW [l]	-
Debranning	-	850KW [l]	-
Liquefaction	184% (v/w) Litres/ kg corn [i] (assume similar to wheat)	89KW [k]	10.6 t/h [k]
Saccharification	-	29.8KW [k]	-
Fermenter	-	159.1 KW [k]	-
Centrifugation 1	-	331.8 KW (assume similar to Rotary Dryer (1))	-
Ethanol recovery	-	51 KW [k]	25 t/h [k]
Washing 1	300% (assumed)	-	-

Utility Requirements (2)

Equipment	Utilities		
	Process water	**Electricity**	**Steam**
Treatment 1	-	29.8KW (assume similar to Saccharification)	1.05 t/h [m]
Treatment 2	1143% [j]	29.8KW (assume similar to Saccharification)	0.49 t/h [m]
Treatment 3	2000% [j]	29.8KW (assume similar to Saccharification)	2.58 t/h [m]
Treatment 4	10,000% [j]		9.86 t/h [m]
Sieving & Washing 2	300% [j]	-	-
Sieving & Washing 3	300% [j]	-	-
Centrifugation 2	-	15.84KW (scaled down from centrifugation (1) based on flowrate)	-
Rotary Dryer 1	-	331.8 KW [k]	-
Rotary Dryer 2	-	331.8 KW (assume similar to Rotary Dryer (1))	-
CO2 Recovery	-	1167KW [m]	-

Utility Requirements (3)

Equipment	Utilities		
	Natural Gas	**Cooling Water**	**Refrigeration**
Saccharification	-	121.93 t/h [k]	-
Fermenter	-	417.07 t/h [k]	-
Treatment 3		119.07 t/h [k]	-
Treatment 4		455.45 t/h [k]	
Precipitation	-	-	219.82 MJ/h [m]
Rotary Dryer 1	0.7 t/h [i]	-	-
Rotary Dryer 2	3.43 MBtu/h [m]	-	-

Please note that the above values have been scaled up/down from the reference value according to flowrate

Source

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f. Keim C.R. and Venkatasubramanian K., 1989. Economics of current biotechnological methods of producing ethanol. *Trends in Biotechnology*, 7, 2, 22.
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h. Mustafa M.A., Washbrook J., Lim J., Zhou Y., Titchener-Hooker N.J., Morton P., Berezenko S., and Farid S.S., 2004. A software tool to assist business-process decision making in the biopharmaceutical industry. *Biotech Progress*, 20, 4, 1096.
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j. Hollmann J. and Lindhauer M.G., 2005. Pilot-scale isolation of glucuronoarabinoxylans from wheat bran. *Carbohydrate Polymers*, 59, 225.
k. Anonymous, 2004. Shelled corn to ethanol process analysis: Dry grind starch fermentation. Agriculture Research Agency of the US Department of Agriculture
l. Satake Corporation UK Division
m. Aspen HYSYS simulations (scaled up/down form HYSYS simulations. Please note that the value depends on flowrate)

Model Assumptions

General assumptions

a. Wheat and bran composition are on dry basis
b. Data for raw material loading based on corn is assumed to be equally valid for wheat
c. If density is unknown, a raw material loading based on volume/volume is assumed similar on a weight/weight

Saccharification

a. Water is consumed in this step to form glucose from starch and hence there is an assumption that the total water reduces by the difference in mass balance between dextrin and glucose to compensate for water losses

Centrifugation

a. The wet grain is assumed to come out at 37% solids
b. The ethanol yield in the product stream has been fixed in the model at 98%

Washing steps

a. Following washing with ethanol, 5% is assumed to be retained by the solids
b. Following washing, 5% of water is retained except in Washing 2 where 20% is left. The reason is that to maintain a final moisture content of about 2% in AX product, otherwise with the previous assumption of 5%, it might result in –ve values

Treatment

a. Assume no ethanol losses in Treatment steps 1-4

DDGS dryer

a. Assume the only overall loss of ethanol is in this step

Arabinoxylan

a. Assume the final product purity is fixed and that everything is wasted in the dryer in order to meet those specific compositions as shown below

	Starch	Protein	Miscellaneous	Moisture
70% Arabinoxylan	0%	11%	17%	2%
80% AX Arabinoxylan	0%	8%	10%	2%

Aspen HYSYS simulation

a. Simulations are conducted, based on the flowrate obtained from Excel, assuming that the stream is a liquid streams only (even if it contains solids). Hence, the impact of the presence of different components (starch, protein, arabinoxylan, miscellaneous) on boiling temperatures, etc, is not considered
b. The duty calculated is the duty required to bring the liquid to the specified temperature. Any extra duty to compensate for heat losses is not included

Appendix C
Equipment Purchase Costs

Appendix C provides the tables of the Purchased Costs of each piece of equipment for all the flowsheets, of the rigorous SuperPro Designer simulations. Flowsheet 1 is the wheat-to-ethanol base case (Tables C1 and C2). Flowsheet 2 is the AX co-production using hammer milling and sieving (Tables C3 and C4), and Flowsheet 3 is the AX co-production using debranner (Tables C5 and C6).

Table C1. Flowsheet 1 Equipment sizing and Purchase Cost (2006 prices in $).

Quantity/ Standby/ Staggered	**Name**	**Description**	**Unit Cost ($)**	**Cost ($)**
1 / 0 / 0	602U	Evaporator	2,528,000	2,528,000
		Evaporation Area = 1228.77 m2		
1 / 0 / 0	103U	Belt Conveyor	98,000	98,000
		Belt Length = 100.00 m		
1 / 0 / 0	104T	Silo/Bin	820,000	820,000
		Vessel Volume = 17462.10 m3		
1 / 0 / 0	101U	Component Splitter	51,000	51,000
		Size/Capacity = 43655.25 kg/h		
1 / 0 / 0	102U	Grinder	83,000	83,000
		Size/Capacity = 43524.29 kg/h		
1 / 0 / 0	202T	Receiver Tank	27,000	27,000
		Vessel Volume = 95.39 m3		
1 / 0 / 0	203T	Hopper	43,000	43,000
		Vessel Volume = 95061.43 L		
1 / 0 / 0	204T	Receiver Tank	36,000	36,000
		Vessel Volume = 95.39 m3		
1 / 0 / 0	217T/TA	Blending Tank	123,000	123,000
		Vessel Volume = 53.77 m3		
1 / 0 / 0	224T	Hopper	8,000	8,000
		Vessel Volume = 4.02 m3		
1 / 0 / 0	218T	Receiver Tank	25,000	25,000
		Vessel Volume = 8.49 m3		
1 / 0 / 0	219T	Receiver Tank	43,000	43,000
		Vessel Volume = 11.81 m3		
1 / 0 / 0	219TP	Gear Pump	3,000	3,000
		Power = 0.20 kW		
1 / 0 / 0	221T/TA	Blending Tank	146,000	146,000
		Vessel Volume = 155.34 m3		
2 / 0 / 0	222T/TA	Stirred Reactor	194,000	388,000
		Vessel Volume = 463.10 m3		
1 / 0 / 0	220T	Receiver Tank	73,000	73,000
		Vessel Volume = 601.38 ft3		
1 / 0 / 0	216T	Receiver Tank	11,000	11,000
		Vessel Volume = 18.28 m3		
1 / 0 / 0	510E	Heat Exchanger	351,000	351,000
		Heat Exchange Area = 426.15 m2		
1 / 0 / 0	405E	Heat Exchanger	202,000	202,000
		Heat Exchange Area = 316.38 m2		
1 / 0 / 0	411P	Gear Pump	5,000	5,000
		Power = 0.05 kW		
6 / 0 / 0	404T/TA	Fermenter	411,000	2,466,000
		Vessel Volume = 2181.75 m3		
1 / 0 / 0	415PT	Absorber	85,000	85,000
		Absorber Volume = 13.41 m3		
1 / 0 / 0	408P	Centrifugal Pump	4,000	4,000
		Power = 2.17 HP		

1 / 0 / 0	508E	Heat Exchanger	436,000	436,000
		Heat Exchange Area = 5331.42 ft2		
1 / 0 / 0	609T	Receiver Tank	87,000	87,000
		Vessel Volume = 588.60 m3		
1 / 0 / 0	407P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	502TT	Distillation Column	497,000	497,000
		Column Volume = 86.73 m3		
1 / 0 / 0	MX-101	Mixer	0	0
		Size/Capacity = 29210.22 kg/h		
1 / 0 / 0	503TT	Distillation Column	220,000	220,000
		Column Volume = 113.57 m3		
1 / 0 / 0	504TT	Distillation Column	137,000	137,000
		Column Volume = 3.23 m3		
1 / 0 / 0	703T	Flat Bottom Tank	81,000	81,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	705T	Flat Bottom Tank	52,000	52,000
		Vessel Volume = 11980.00 ft3		
1 / 0 / 0	704T	Flat Bottom Tank	251,000	251,000
		Vessel Volume = 3392.22 m3		
1 / 0 / 0	607T	Blending Tank	171,000	171,000
		Vessel Volume = 755.41 m3		
1 / 0 / 0	601U	Decanter Centrifuge	1,348,000	1,348,000
		Throughput = 2143.08 L/min		
1 / 0 / 0	608T	Blending Tank	199,000	199,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	611U	Belt Conveyor	46,000	46,000
		Belt Length = 100.00 m		
1 / 0 / 0	MX-102	Mixer	0	0
		Size/Capacity = 40657.95 kg/h		
1 / 0 / 0	603U	Rotary Dryer	1,027,000	1,027,000
		Drying Area = 1130.38 m2		
1 / 0 / 0	612U	Belt Conveyor	100,000	100,000
		Belt Length = 100.00 m		
1 / 0 / 0	MX-103	Mixer	0	0
		Size/Capacity = 12898.34 kg/h		
1 / 0 / 0	MX-104	Mixer	0	0
		Size/Capacity = 151332.86 kg/h		
1 / 0 / 0	207E	Heat Exchanger	64,000	64,000
		Heat Exchange Area = 610.77 ft2		
1 / 0 / 0	206E	Heat Exchanger	191,000	191,000
		Heat Exchange Area = 4759.81 ft2		
1 / 0 / 0	BS-MIX	Mixer	0	0
		Size/Capacity = 164030.99 kg/h		
1 / 0 / 0	218TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	220TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	216TP	Gear Pump	3,000	3,000
		Power = 0.02 kW		
1 / 0 / 0	414T/TP	Blending Tank	103,000	103,000
		Vessel Volume = 2.91 m3		
1 / 0 / 0	610U	Wet Air Oxidizer	930,000	930,000
		Vessel Volume = 11.54 m3		
1 / 0 / 0	525P	Gear Pump	5,000	5,000
		Power = 1.61 HP		
1 / 0 / 0	702P	Gear Pump	5,000	5,000
		Power = 5.00 HP		
1 / 0 / 0	FSP-103	Flow Splitter	0	0
		Size/Capacity = 96696.92 kg/h		

4 / 0 / 0	403E	Heat Exchanger	60,000	240,000
		Heat Exchange Area = 1000.00 ft2		
3 / 0 / 0	223V	Receiver Tank	51,000	153,000
		Vessel Volume = 14.16 m3		
2 / 0 / 0	501V	Flash Drum	28,000	56,000
		Vessel Volume = 540.51 ft3		
1 / 0 / 0	507E	Condenser	84,000	84,000
		Condensation Area = 670.01 ft2		
1 / 0 / 0	FSP-102	Flow Splitter	0	0
		Size/Capacity = 151538.73 kg/h		
1 / 0 / 0	511E	Heat Exchanger	563,000	563,000
		Heat Exchange Area = 6065.15 ft2		
3 / 0 / 0	211P	Centrifugal Pump	36,000	108,000
		Power = 100.00 HP		
1 / 0 / 0	212P	Centrifugal Pump	12,000	12,000
		Power = 50.00 kW		
1 / 0 / 0	213P	Centrifugal Pump	13,000	13,000
		Power = 50.00 HP		
4 / 1 / 0	402P	Centrifugal Pump	13,000	65,000
		Power = 10.96 HP		
1 / 1 / 0	409P	Centrifugal Pump	13,000	26,000
		Power = 25.20 HP		
1 / 0 / 0	512P	Centrifugal Pump	4,000	4,000
		Power = 50.00 HP		
1 / 0 / 0	513P	Centrifugal Pump	4,000	4,000
		Power = 20.00 HP		
1 / 0 / 0	514P	Centrifugal Pump	4,000	4,000
		Power = 10.00 HP		
1 / 0 / 0	515P	Centrifugal Pump	3,000	3,000
		Power = 0.78 HP		
1 / 0 / 0	604P	Centrifugal Pump	10,000	10,000
		Power = 20.00 HP		
1 / 0 / 0	605P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	606P	Centrifugal Pump	10,000	10,000
		Power = 20.00 HP		
1 / 0 / 0	701U	Centrifugal Pump	28,000	28,000
		Power = 10.00 HP		
1 / 0 / 0	406E	Heat Exchanger	32,000	32,000
		Heat Exchange Area = 1928.00 ft2		
1 / 0 / 0	MX-105	Mixer	0	0
		Size/Capacity = 13442.67 kg/h		
1 / 0 / 0	205E	Heat Exchanger	15,000	15,000
		Heat Exchange Area = 713.29 ft2		
1 / 0 / 0	517U	Generic Box	1,320,000	1,320,000
		Size/Capacity = 16356.40 kg/h		
1 / 0 / 0	MX-106	Mixer	0	0
		Size/Capacity = 43655.25 kg/h		
1 / 0 / 0	FSP-101	Flow Splitter	0	0
		Size/Capacity = 86422.75 kg/h		
1 / 0 / 0	MX-107	Mixer	0	0
		Size/Capacity = 94948.97 kg/h		
		Unlisted Equipment		0
			TOTAL	16,362,000

Table C2. Flowsheet 1 Direct Fixed Capital (DFC) Summary (2006 prices in $).

Section Name	**DFC ($)**
Grain Handling & Milling	3,197,000
Starch to Sugar Conversion	6,589,000
Fermentation	12,092,000
Ethanol Processing	8,173,000
Co-Product Processing	20,597,000
Common Support Systems	600,000
Plant DFC	51,248,000

Table C3. Flowsheet 2 Equipment sizing and Purchase Cost (2006 prices in $).

Quantity/ Standby/ Staggered	**Name**	**Description**	**Unit Cost ($)**	**Cost ($)**
1 / 0 / 0	602U	Evaporator	2,522,000	2,522,000
		Evaporation Area = 1223.45 m2		
1 / 0 / 0	103U	Belt Conveyor	98,000	98,000
		Belt Length = 100.00 m		
1 / 0 / 0	104T	Silo/Bin	819,000	819,000
		Vessel Volume = 17430.84 m3		
1 / 0 / 0	101U	Component Splitter	51,000	51,000
		Size/Capacity = 43577.10 kg/h		
1 / 0 / 0	102U	Grinder	83,000	83,000
		Size/Capacity = 43446.37 kg/h		
1 / 0 / 0	202T	Receiver Tank	26,000	26,000
		Vessel Volume = 89.71 m3		
1 / 0 / 0	203T	Hopper	41,000	41,000
		Vessel Volume = 90547.39 L		
1 / 0 / 0	204T	Receiver Tank	35,000	35,000
		Vessel Volume = 89.71 m3		
1 / 0 / 0	217T/TA	Blending Tank	122,000	122,000
		Vessel Volume = 52.62 m3		
1 / 0 / 0	224T	Hopper	8,000	8,000
		Vessel Volume = 4.02 m3		
1 / 0 / 0	218T	Receiver Tank	25,000	25,000
		Vessel Volume = 8.49 m3		
1 / 0 / 0	219T	Receiver Tank	43,000	43,000
		Vessel Volume = 11.81 m3		
1 / 0 / 0	219TP	Gear Pump	3,000	3,000
		Power = 0.20 kW		
1 / 0 / 0	221T/TA	Blending Tank	144,000	144,000
		Vessel Volume = 152.04 m3		
2 / 0 / 0	222T/TA	Stirred Reactor	192,000	384,000
		Vessel Volume = 455.27 m3		
1 / 0 / 0	220T	Receiver Tank	73,000	73,000
		Vessel Volume = 601.38 ft3		
1 / 0 / 0	216T	Receiver Tank	11,000	11,000
		Vessel Volume = 18.28 m3		
1 / 0 / 0	510E	Heat Exchanger	341,000	341,000
		Heat Exchange Area = 405.39 m2		
1 / 0 / 0	405E	Heat Exchanger	202,000	202,000
		Heat Exchange Area = 307.88 m2		
1 / 0 / 0	411P	Gear Pump	5,000	5,000
		Power = 0.05 kW		
6 / 0 / 0	404T/TA	Fermenter	407,000	2,442,000
		Vessel Volume = 2144.06 m3		
1 / 0 / 0	415PT	Absorber	85,000	85,000

		Absorber Volume = 13.41 m3		
1 / 0 / 0	408P	Centrifugal Pump	4,000	4,000
		Power = 2.17 HP		
1 / 0 / 0	508E	Heat Exchanger	436,000	436,000
		Heat Exchange Area = 5261.63 ft2		
1 / 0 / 0	609T	Receiver Tank	88,000	88,000
		Vessel Volume = 604.05 m3		
1 / 0 / 0	407P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	502TT	Distillation Column	494,000	494,000
		Column Volume = 85.76 m3		
1 / 0 / 0	503TT	Distillation Column	285,000	285,000
		Column Volume = 117.63 m3		
1 / 0 / 0	504TT	Distillation Column	153,000	153,000
		Column Volume = 3.91 m3		
1 / 0 / 0	703T	Flat Bottom Tank	81,000	81,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	705T	Flat Bottom Tank	52,000	52,000
		Vessel Volume = 11980.00 ft3		
1 / 0 / 0	704T	Flat Bottom Tank	251,000	251,000
		Vessel Volume = 3392.22 m3		
1 / 0 / 0	607T	Blending Tank	171,000	171,000
		Vessel Volume = 755.41 m3		
1 / 0 / 0	601U	Decanter Centrifuge	1,322,000	1,322,000
		Throughput = 2101.67 L/min		
1 / 0 / 0	608T	Blending Tank	199,000	199,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	611U	Belt Conveyor	46,000	46,000
		Belt Length = 100.00 m		
1 / 0 / 0	MX-102	Mixer	0	0
		Size/Capacity = 39153.21 kg/h		
1 / 0 / 0	603U	Rotary Dryer	1,027,000	1,027,000
		Drying Area = 1131.46 m2		
1 / 0 / 0	612U	Belt Conveyor	100,000	100,000
		Belt Length = 100.00 m		
1 / 0 / 0	MX-103	Mixer	0	0
		Size/Capacity = 12855.48 kg/h		
1 / 0 / 0	MX-104	Mixer	0	0
		Size/Capacity = 149127.92 kg/h		
1 / 0 / 0	207E	Heat Exchanger	62,000	62,000
		Heat Exchange Area = 590.83 ft2		
1 / 0 / 0	206E	Heat Exchanger	190,000	190,000
		Heat Exchange Area = 4722.80 ft2		
1 / 0 / 0	BS-MIX	Mixer	0	0
		Size/Capacity = 161790.98 kg/h		
1 / 0 / 0	218TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	220TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	216TP	Gear Pump	3,000	3,000
		Power = 0.02 kW		
1 / 0 / 0	414T/TP	Blending Tank	103,000	103,000
		Vessel Volume = 2.91 m3		
1 / 0 / 0	610U	Wet Air Oxidizer	930,000	930,000
		Vessel Volume = 11.55 m3		
1 / 0 / 0	525P	Gear Pump	5,000	5,000
		Power = 1.57 HP		
1 / 0 / 0	702P	Gear Pump	5,000	5,000
		Power = 5.00 HP		
1 / 0 / 0	FSP-103	Flow Splitter	0	0

		Size/Capacity = 95842.55 kg/h		
4 / 0 / 0	403E	Heat Exchanger	60,000	240,000
		Heat Exchange Area = 1000.00 ft2		
3 / 0 / 0	223V	Receiver Tank	51,000	153,000
		Vessel Volume = 14.16 m3		
2 / 0 / 0	501V	Flash Drum	28,000	56,000
		Vessel Volume = 532.64 ft3		
1 / 0 / 0	507E	Condenser	84,000	84,000
		Condensation Area = 665.72 ft2		
1 / 0 / 0	FSP-102	Flow Splitter	0	0
		Size/Capacity = 149340.60 kg/h		
1 / 0 / 0	511E	Heat Exchanger	559,000	559,000
		Heat Exchange Area = 6006.80 ft2		
3 / 0 / 0	211P	Centrifugal Pump	36,000	108,000
		Power = 100.00 HP		
1 / 0 / 0	212P	Centrifugal Pump	12,000	12,000
		Power = 50.00 kW		
1 / 0 / 0	213P	Centrifugal Pump	13,000	13,000
		Power = 50.00 HP		
4 / 1 / 0	402P	Centrifugal Pump	13,000	65,000
		Power = 10.96 HP		
1 / 1 / 0	409P	Centrifugal Pump	13,000	26,000
		Power = 25.20 HP		
1 / 0 / 0	512P	Centrifugal Pump	4,000	4,000
		Power = 50.00 HP		
1 / 0 / 0	513P	Centrifugal Pump	4,000	4,000
		Power = 20.00 HP		
1 / 0 / 0	514P	Centrifugal Pump	4,000	4,000
		Power = 10.00 HP		
1 / 0 / 0	604P	Centrifugal Pump	10,000	10,000
		Power = 20.00 HP		
1 / 0 / 0	605P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	606P	Centrifugal Pump	10,000	10,000
		Power = 20.00 HP		
1 / 0 / 0	701U	Centrifugal Pump	28,000	28,000
		Power = 10.00 HP		
1 / 0 / 0	406E	Heat Exchanger	32,000	32,000
		Heat Exchange Area = 1928.00 ft2		
1 / 0 / 0	MX-105	Mixer	0	0
		Size/Capacity = 13106.56 kg/h		
1 / 0 / 0	205E	Heat Exchanger	17,000	17,000
		Heat Exchange Area = 800.32 ft2		
1 / 0 / 0	517U	Generic Box	1,302,000	1,302,000
		Size/Capacity = 15979.26 kg/h		
1 / 0 / 0	MX-106	Mixer	0	0
		Size/Capacity = 43577.10 kg/h		
1 / 0 / 0	FSP-101	Flow Splitter	0	0
		Size/Capacity = 88648.60 kg/h		
1 / 0 / 0	MX-107	Mixer	0	0
		Size/Capacity = 95000.00 kg/h		
1 / 0 / 0	HX-101	Heat Exchanger	40,000	40,000
		Heat Exchange Area = 6.57 m2		
1 / 0 / 0	DDR-101	Drum Dryer	904,000	904,000
		Drum Area = 31.80 m2		
1 / 0 / 0	MX-109	Mixer	0	0
		Size/Capacity = 18303.01 kg/h		
1 / 0 / 0	V-102	Blending Tank	37,000	37,000
		Vessel Volume = 40675.65 L		
1 / 0 / 0	MX-110	Mixer	0	0

		Size/Capacity = 29290.07 kg/h		
1 / 0 / 0	V-103	Blending Tank	55,000	55,000
		Vessel Volume = 129.34 m3		
1 / 0 / 0	HX-102	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 1.70 m2		
1 / 0 / 0	HX-103	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 0.46 m2		
1 / 0 / 0	V-101	Blending Tank	41,000	41,000
		Vessel Volume = 63360.31 L		
1 / 0 / 0	MX-111	Mixer	0	0
		Size/Capacity = 29582.97 kg/h		
1 / 0 / 0	MX-112	Mixer	0	0
		Size/Capacity = 29588.89 kg/h		
1 / 0 / 0	V-104	Blending Tank	113,000	113,000
		Vessel Volume = 391.37 m3		
1 / 0 / 0	HX-104	Heat Exchanger	30,000	30,000
		Heat Exchange Area = 14.16 m2		
1 / 0 / 0	V-105	Blending Tank	18,000	18,000
		Vessel Volume = 8393.76 L		
1 / 0 / 0	HX-105	Heat Exchanger	35,000	35,000
		Heat Exchange Area = 13.56 m2		
1 / 0 / 0	MX-113	Mixer	0	0
		Size/Capacity = 29884.78 kg/h		
1 / 0 / 0	MX-114	Mixer	0	0
		Size/Capacity = 29890.76 kg/h		
1 / 0 / 0	MX-115	Mixer	0	0
		Size/Capacity = 30189.66 kg/h		
1 / 0 / 0	MX-116	Mixer	0	0
		Size/Capacity = 30195.70 kg/h		
1 / 0 / 0	V-108	Flat Bottom Tank	55,000	55,000
		Vessel Volume = 72760.34 L		
1 / 0 / 0	DC-101	Decanter Centrifuge	207,000	207,000
		Throughput = 3337.35 L/h		
1 / 0 / 0	DDR-102	Drum Dryer	446,000	446,000
		Drum Area = 12.70 m2		
1 / 0 / 0	MX-101	Mixer	0	0
		Size/Capacity = 42855.78 kg/h		
1 / 0 / 0	CSP-102	Component Splitter	26,000	26,000
		Size/Capacity = 11598.50 kg/h		
1 / 0 / 0	CSP-103	Component Splitter	26,000	26,000
		Size/Capacity = 18303.01 kg/h		
1 / 0 / 0	HX-106	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 1.28 m2		
1 / 0 / 0	CSP-104	Component Splitter	32,000	32,000
		Size/Capacity = 30195.70 kg/h		
1 / 0 / 0	CSP-105	Component Splitter	200,000	200,000
		Size/Capacity = 25601.83 kg/h		
1 / 0 / 0	FSP-105	Flow Splitter	0	0
		Size/Capacity = 11185.48 kg/h		
1 / 0 / 0	MX-108	Mixer	0	0
		Size/Capacity = 11598.50 kg/h		
1 / 0 / 0	MX-117	Mixer	0	0
		Size/Capacity = 4058.14 kg/h		
1 / 0 / 0	V-106	Blending Tank	35,000	35,000
		Vessel Volume = 32913.30 L		
1 / 0 / 0	V-107	Blending Tank	20,000	20,000
		Vessel Volume = 11071.99 L		
1 / 0 / 0	FSP-104	Flow Splitter	0	0
		Size/Capacity = 27164.74 kg/h		
1 / 0 / 0	PM-101	Centrifugal Pump	11,000	11,000

		Power = 0.57 kW		
1 / 0 / 0	CSP-106	Component Splitter	40,000	40,000
		Size/Capacity = 4058.14 kg/h		
1 / 0 / 0	HX-107	Heat Exchanger	2,000	2,000
		Heat Exchange Area = 3.30 m2		
1 / 0 / 0	HX-108	Heat Exchanger	18,000	18,000
		Heat Exchange Area = 22.62 m2		
1 / 0 / 0	MX-119	Mixer	0	0
		Size/Capacity = 13570.01 kg/h		
1 / 0 / 0	CSP-101	Component Splitter	0	0
		Size/Capacity = 43446.37 kg/h		
1 / 0 / 0	MX-120	Mixer	0	0
		Size/Capacity = 21877.37 kg/h		
3 / 0 / 0	V-109	Blending Tank	100,000	300,000
		Vessel Volume = 322.53 m3		
1 / 0 / 0	MX-121	Mixer	0	0
		Size/Capacity = 73667.98 kg/h		
1 / 0 / 0	CSP-107	Component Splitter	0	0
		Size/Capacity = 21877.37 kg/h		
1 / 0 / 0	FSP-106	Flow Splitter	0	0
		Size/Capacity = 508.13 kg/h		
		Unlisted Equipment		145,000
			TOTAL	19,246,000

Table C4. Flowsheet 2 Direct Fixed Capital (DFC) Summary (2006 prices in $).

Section Name	**DFC ($)**
Grain Handling & Milling	3,182,000
Starch to Sugar Conversion	6,550,000
Fermentation	11,987,000
Ethanol Processing	8,321,000
Co-Product Processing	20,502,000
Common Support Systems	600,000
Arabinoxylans Production	10,183,000
Plant DFC	61,326,000

Table C5. Flowsheet 2 Equipment sizing and Purchase Cost (2006 prices in $).

Quantity/ Standby/ Staggered	**Name**	**Description**	**Unit Cost ($)**	**Cost ($)**
1 / 0 / 0	602U	Evaporator	2,522,000	2,522,000
		Evaporation Area = 1223.89 m2		
1 / 0 / 0	103U	Belt Conveyor	98,000	98,000
		Belt Length = 100.00 m		
1 / 0 / 0	104T	Silo/Bin	819,000	819,000
		Vessel Volume = 17430.84 m3		
1 / 0 / 0	101U	Component Splitter	51,000	51,000
		Size/Capacity = 43577.10 kg/h		
1 / 0 / 0	102U	Grinder	81,000	81,000
		Size/Capacity = 41519.34 kg/h		
1 / 0 / 0	202T	Receiver Tank	26,000	26,000
		Vessel Volume = 3171.66 ft3		
1 / 0 / 0	203T	Hopper	42,000	42,000
		Vessel Volume = 90682.42 L		
1 / 0 / 0	204T	Receiver Tank	35,000	35,000
		Vessel Volume = 89.81 m3		
1 / 0 / 0	217T/TA	Blending Tank	122,000	122,000

		Vessel Volume = 52.68 m3		
1 / 0 / 0	224T	Hopper	8,000	8,000
		Vessel Volume = 4.02 m3		
1 / 0 / 0	218T	Receiver Tank	25,000	25,000
		Vessel Volume = 8.49 m3		
1 / 0 / 0	219T	Receiver Tank	43,000	43,000
		Vessel Volume = 11.81 m3		
1 / 0 / 0	219TP	Gear Pump	3,000	3,000
		Power = 0.20 kW		
1 / 0 / 0	221T/TA	Blending Tank	145,000	145,000
		Vessel Volume = 152.19 m3		
2 / 0 / 0	222T/TA	Stirred Reactor	192,000	384,000
		Vessel Volume = 456.57 m3		
1 / 0 / 0	220T	Receiver Tank	73,000	73,000
		Vessel Volume = 601.38 ft3		
1 / 0 / 0	216T	Receiver Tank	11,000	11,000
		Vessel Volume = 18.28 m3		
1 / 0 / 0	510E	Heat Exchanger	389,000	389,000
		Heat Exchange Area = 5436.25 ft2		
1 / 0 / 0	405E	Heat Exchanger	202,000	202,000
		Heat Exchange Area = 310.41 m2		
1 / 0 / 0	411P	Gear Pump	5,000	5,000
		Power = 0.05 kW		
6 / 0 / 0	404T/TA	Fermenter	407,000	2,442,000
		Vessel Volume = 2144.88 m3		
1 / 0 / 0	415PT	Absorber	85,000	85,000
		Absorber Volume = 13.41 m3		
1 / 0 / 0	408P	Centrifugal Pump	4,000	4,000
		Power = 2.17 HP		
1 / 0 / 0	508E	Heat Exchanger	436,000	436,000
		Heat Exchange Area = 5262.83 ft2		
1 / 0 / 0	609T	Receiver Tank	0	0
		Vessel Volume = 0.02 m3		
1 / 0 / 0	407P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	502TT	Distillation Column	494,000	494,000
		Column Volume = 85.82 m3		
1 / 0 / 0	503TT	Distillation Column	220,000	220,000
		Column Volume = 113.57 m3		
1 / 0 / 0	504TT	Distillation Column	156,000	156,000
		Column Volume = 4.03 m3		
1 / 0 / 0	703T	Flat Bottom Tank	81,000	81,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	705T	Flat Bottom Tank	52,000	52,000
		Vessel Volume = 11980.00 ft3		
1 / 0 / 0	704T	Flat Bottom Tank	251,000	251,000
		Vessel Volume = 3392.22 m3		
1 / 0 / 0	607T	Blending Tank	171,000	171,000
		Vessel Volume = 755.41 m3		
1 / 0 / 0	601U	Decanter Centrifuge	1,323,000	1,323,000
		Throughput = 2102.30 L/min		
1 / 0 / 0	608T	Blending Tank	199,000	199,000
		Vessel Volume = 481.39 m3		
1 / 0 / 0	611U	Belt Conveyor	46,000	46,000
		Belt Length = 100.00 m		
1 / 0 / 0	MX-102	Mixer	0	0
		Size/Capacity = 39174.55 kg/h		
1 / 0 / 0	603U	Rotary Dryer	1,027,000	1,027,000
		Drying Area = 1131.73 m2		
1 / 0 / 0	612U	Belt Conveyor	100,000	100,000

		Belt Length = 100.00 m		
1 / 0 / 0	MX-103	Mixer	0	0
		Size/Capacity = 12857.64 kg/h		
1 / 0 / 0	MX-104	Mixer	0	0
		Size/Capacity = 149187.87 kg/h		
1 / 0 / 0	207E	Heat Exchanger	62,000	62,000
		Heat Exchange Area = 591.06 ft2		
1 / 0 / 0	206E	Heat Exchanger	190,000	190,000
		Heat Exchange Area = 4723.88 ft2		
1 / 0 / 0	BS-MIX	Mixer	0	0
		Size/Capacity = 161843.36 kg/h		
1 / 0 / 0	218TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	220TP	Gear Pump	3,000	3,000
		Power = 0.25 HP		
1 / 0 / 0	216TP	Gear Pump	3,000	3,000
		Power = 0.02 kW		
1 / 0 / 0	414T/TP	Blending Tank	103,000	103,000
		Vessel Volume = 2.91 m3		
1 / 0 / 0	610U	Wet Air Oxidizer	930,000	930,000
		Vessel Volume = 11.56 m3		
1 / 0 / 0	525P	Gear Pump	5,000	5,000
		Power = 1.56 HP		
1 / 0 / 0	702P	Gear Pump	5,000	5,000
		Power = 5.00 HP		
1 / 0 / 0	FSP-103	Flow Splitter	0	0
		Size/Capacity = 95806.61 kg/h		
4 / 0 / 0	403E	Heat Exchanger	60,000	240,000
		Heat Exchange Area = 1000.00 ft2		
3 / 0 / 0	223V	Receiver Tank	51,000	153,000
		Vessel Volume = 14.16 m3		
2 / 0 / 0	501V	Flash Drum	28,000	56,000
		Vessel Volume = 532.85 ft3		
1 / 0 / 0	507E	Condenser	84,000	84,000
		Condensation Area = 666.16 ft2		
1 / 0 / 0	FSP-102	Flow Splitter	0	0
		Size/Capacity = 149390.12 kg/h		
1 / 0 / 0	511E	Heat Exchanger	480,000	480,000
		Heat Exchange Area = 4964.29 ft2		
3 / 0 / 0	211P	Centrifugal Pump	36,000	108,000
		Power = 100.00 HP		
1 / 0 / 0	212P	Centrifugal Pump	12,000	12,000
		Power = 50.00 kW		
1 / 0 / 0	213P	Centrifugal Pump	13,000	13,000
		Power = 50.00 HP		
4 / 1 / 0	402P	Centrifugal Pump	13,000	65,000
		Power = 10.96 HP		
1 / 1 / 0	409P	Centrifugal Pump	13,000	26,000
		Power = 25.20 HP		
1 / 0 / 0	512P	Centrifugal Pump	4,000	4,000
		Power = 50.00 HP		
1 / 0 / 0	513P	Centrifugal Pump	4,000	4,000
		Power = 20.00 HP		
1 / 0 / 0	514P	Centrifugal Pump	4,000	4,000
		Power = 10.00 HP		
1 / 0 / 0	604P	Centrifugal Pump	10,000	10,000
		Power = 20.00 HP		
1 / 0 / 0	605P	Centrifugal Pump	12,000	12,000
		Power = 50.00 HP		
1 / 0 / 0	606P	Centrifugal Pump	10,000	10,000

		Power = 20.00 HP		
1 / 0 / 0	701U	Centrifugal Pump	28,000	28,000
		Power = 10.00 HP		
1 / 0 / 0	406E	Heat Exchanger	32,000	32,000
		Heat Exchange Area = 1928.00 ft2		
1 / 0 / 0	MX-105	Mixer	0	0
		Size/Capacity = 13069.52 kg/h		
1 / 0 / 0	205E	Heat Exchanger	16,000	16,000
		Heat Exchange Area = 782.88 ft2		
1 / 0 / 0	517U	Generic Box	1,294,000	1,294,000
		Size/Capacity = 15820.05 kg/h		
1 / 0 / 0	MX-106	Mixer	0	0
		Size/Capacity = 43577.10 kg/h		
1 / 0 / 0	FSP-101	Flow Splitter	0	0
		Size/Capacity = 88917.46 kg/h		
1 / 0 / 0	MX-107	Mixer	0	0
		Size/Capacity = 95000.00 kg/h		
1 / 0 / 0	HX-101	Heat Exchanger	40,000	40,000
		Heat Exchange Area = 7.40 m2		
1 / 0 / 0	DDR-101	Drum Dryer	1,429,000	1,429,000
		Drum Area = 57.68 m2		
1 / 0 / 0	MX-109	Mixer	0	0
		Size/Capacity = 19286.17 kg/h		
1 / 0 / 0	V-102	Blending Tank	38,000	38,000
		Vessel Volume = 42869.03 L		
1 / 0 / 0	MX-110	Mixer	0	0
		Size/Capacity = 32245.55 kg/h		
1 / 0 / 0	V-103	Blending Tank	58,000	58,000
		Vessel Volume = 142.51 m3		
1 / 0 / 0	HX-102	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 2.52 m2		
1 / 0 / 0	HX-103	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 0.65 m2		
1 / 0 / 0	V-101	Blending Tank	43,000	43,000
		Vessel Volume = 69217.88 L		
1 / 0 / 0	MX-111	Mixer	0	0
		Size/Capacity = 32568.00 kg/h		
1 / 0 / 0	MX-112	Mixer	0	0
		Size/Capacity = 32574.52 kg/h		
2 / 0 / 0	V-104	Blending Tank	79,000	158,000
		Vessel Volume = 215.58 m3		
1 / 0 / 0	HX-104	Heat Exchanger	30,000	30,000
		Heat Exchange Area = 15.64 m2		
1 / 0 / 0	V-105	Blending Tank	19,000	19,000
		Vessel Volume = 9246.51 L		
1 / 0 / 0	HX-105	Heat Exchanger	35,000	35,000
		Heat Exchange Area = 14.95 m2		
1 / 0 / 0	MX-113	Mixer	0	0
		Size/Capacity = 32900.26 kg/h		
1 / 0 / 0	MX-114	Mixer	0	0
		Size/Capacity = 32906.84 kg/h		
1 / 0 / 0	MX-115	Mixer	0	0
		Size/Capacity = 33235.91 kg/h		
1 / 0 / 0	MX-116	Mixer	0	0
		Size/Capacity = 33242.56 kg/h		
1 / 0 / 0	V-108	Flat Bottom Tank	47,000	47,000
		Vessel Volume = 55220.80 L		
1 / 0 / 0	DC-101	Decanter Centrifuge	207,000	207,000
		Throughput = 2476.27 L/h		
1 / 0 / 0	DDR-102	Drum Dryer	337,000	337,000

		Drum Area = 8.82 m2		
1 / 0 / 0	MX-101	Mixer	0	0
		Size/Capacity = 42888.23 kg/h		
1 / 0 / 0	HX-106	Heat Exchanger	25,000	25,000
		Heat Exchange Area = 1.38 m2		
1 / 0 / 0	CSP-105	Component Splitter	100,000	100,000
		Size/Capacity = 17401.46 kg/h		
1 / 0 / 0	FSP-105	Flow Splitter	0	0
		Size/Capacity = 11074.04 kg/h		
1 / 0 / 0	MX-108	Mixer	0	0
		Size/Capacity = 12709.88 kg/h		
1 / 0 / 0	MX-117	Mixer	0	0
		Size/Capacity = 3066.41 kg/h		
1 / 0 / 0	V-106	Blending Tank	37,000	37,000
		Vessel Volume = 36259.41 L		
1 / 0 / 0	V-107	Blending Tank	21,000	21,000
		Vessel Volume = 12197.54 L		
1 / 0 / 0	FSP-104	Flow Splitter	0	0
		Size/Capacity = 26894.09 kg/h		
1 / 0 / 0	PM-101	Centrifugal Pump	11,000	11,000
		Power = 0.55 kW		
1 / 0 / 0	CSP-106	Component Splitter	40,000	40,000
		Size/Capacity = 3066.41 kg/h		
1 / 0 / 0	HX-107	Heat Exchanger	1,000	1,000
		Heat Exchange Area = 2.60 m2		
1 / 0 / 0	HX-108	Heat Exchanger	56,000	56,000
		Heat Exchange Area = 94.54 m2		
1 / 0 / 0	MX-119	Mixer	0	0
		Size/Capacity = 13647.93 kg/h		
1 / 0 / 0	CSP-101	Component Splitter	1,000,000	1,000,000
		Size/Capacity = 43446.37 kg/h		
1 / 0 / 0	MX-120	Mixer	0	0
		Size/Capacity = 21197.34 kg/h		
3 / 0 / 0	V-109	Blending Tank	98,000	294,000
		Vessel Volume = 312.62 m3		
1 / 0 / 0	MX-121	Mixer	0	0
		Size/Capacity = 77749.22 kg/h		
1 / 0 / 0	CSP-107	Component Splitter	0	0
		Size/Capacity = 21197.34 kg/h		
1 / 0 / 0	MX-118	Mixer	0	0
		Size/Capacity = 9261.76 kg/h		
1 / 0 / 0	FSP-106	Flow Splitter	0	0
		Size/Capacity = 353.00 kg/h		
1 / 0 / 0	PFF-101	Plate & Frame Filter	58,000	58,000
		Filter Area = 21.62 m2		
1 / 0 / 0	PFF-102	Plate & Frame Filter	80,000	80,000
		Filter Area = 31.21 m2		
1 / 0 / 0	PFF-103	Plate & Frame Filter	89,000	89,000
		Filter Area = 35.18 m2		
		Unlisted Equipment		226,000
			TOTAL	20,675,000

Table C6. Flowsheet 3 Direct Fixed Capital (DFC) Summary (2006 prices in $).

Section Name	**DFC ($)**
Main Section	0
Grain Handling & Milling	3,175,000
Starch to Sugar Conversion	6,037,000
Fermentation	12,127,000
Ethanol Processing	8,118,000
Co-Product Processing	20,506,000
Common Support Systems	600,000
Arabinoxylans Production	15,936,000
Plant DFC	66,498,000