FLOWSHEET SIMULATION STUDIES OF NEW OILSEED EXTRACTION PROCESSES

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ABSTRACT

Results are reported on the flowsheet simulation studies of new oilseed processes suitable for local conditions. A process model was developed and new design simulation methods using Computer Aided Design (CAD) approach were employed for the preliminary investigation of a number of alternative scenarios.

Results have shown that new processes should give considerable investment savings if separation of the crude product is not carried out by distillation. However, the economics of processes using alternative separation technology is highly dependent on operating conditions.

The use of spreadsheet programs for flowsheet evaluation studies offers opportunities for application of CAD techniques in local design teams as an effective tool for preliminary process analysis, planning and evaluation.

INTRODUCTION

The importance of agriculture in less developing countries cannot be overemphasized. Future industrialization in these countries should be based on indigenous agricultural resources such as oilseed processing. Processes for the extraction of oils from vegetable seeds could form the starting point of a network of related and economically linked industries that use crude vegetable oils to produce refined oils, margarines, products based on hydrogenated vegetable oils, fatty acids, soaps and detergents and also processes to produce edible protein meal left after extraction of oil.

In Tanzania, existing processes used for recovery of oil are inefficient utilizing near obsolete technology. These plants are mainly mechanical expression plants. In most cases, these plants operate below designed capacities. For example, typical production capacities for MOPROCO range between 30% to 50% of the designed valves.

Although it is known that oilseeds form the natural raw material basis for the establishment of a modern, technically and economically up to date vegetable oil industry, the great potential of oilseeds is still not being fully exploited in Tanzania. There have been local attempts to improve efficiencies of existing mills in two main approaches. First. by improving production capacities of existing mechanical expression plants and second, by installation of solvent extraction plants which will utilize the prepressed cakes produced by expression plants. Another objective has been to improve by-products for use as food or animal feedstocks.

Improvement of production capacities of mechanical expression plants can be attained by careful control of preprocessing operations such as dehulling and conditioning of the seeds. In most plants expression operating conditions cannot be easily adjusted to wide range of the seeds processed. At MOPROCO a solvent extraction plant designed to process 125 tonnes per day prepressed cake containing 12.5% oil by weight has been installed. However plant startup has been delayed because of lack of hexane, lack of trained operators and inappropriate quality control which raise significant safety questions. The continuous operation of this plant will require import of the solvent (hexane) from abroad.

Although attempts have been made in the past to increase efficiency of existing oilseed capacities, new design approaches are essential which will utilize developments in process design technology. These new processes will use solvents produced from indigenous raw materials. This research is directed towards the investigation of these new processes and deals with the details of flowsheet simulation studies of the new oilseed extraction flowsheets. Attention has been paid to integration of raw material resources and the constraints of local distribution, marketing and operator skills. A further objective of this work is to investigate the suitability of the Computer Aided Design approach used for local design teams.

FLOWSHEET SIMULATION IN PROCESS DESIGN

Westerberg et al. (1979) has defined flowsheet simulation, also known as steady state chemical process simulation, as the use of computer aids to perform steady state heat and mass balancing, sizing and costing calculations for a chemical process. The use of computers in chemical process design is now wide spread. With the increasing availability of flowsheeting software which is easy to use with a minimum of additional programming effort, a large number of alternative scenarios can be investigated when a new manufacturing facility is proposed. During the preliminary design stage of a project, the aim is to compare a large number of prepared flowsheets as quickly and as cheaply as possible to highlight the most promising alternatives for further detailed study. This involves repetitive calculations and, if the flowsheet is complicated by recycle, as is the case with oilseed process flowsheet, the iterative calculations can be tedious and error-prone.

With the increasing power of large computers in the early sixties, large flowsheeting programs were developed which enabled calculations on entire flowsheets to be performed. Several general purpose sequential flowsheeting programs have been developed and a number of reviews of existing software are available including those of Flower and Whitehead (1973), and also of Motard et al. (1975). This is still the trend today. Since 1978, PC-Based programs have been also developed that gives the user a large grid of cells into which numbers and formulae can be entered. These programs, known as spreadsheets, are now widely used in a range of chemical engineering applications including flowsheet simulations as noted by Rosen and Adams (1987).

USING THE SPREADSHEET PROGRAM FOR FLOWSHEET CALCULATIONS.

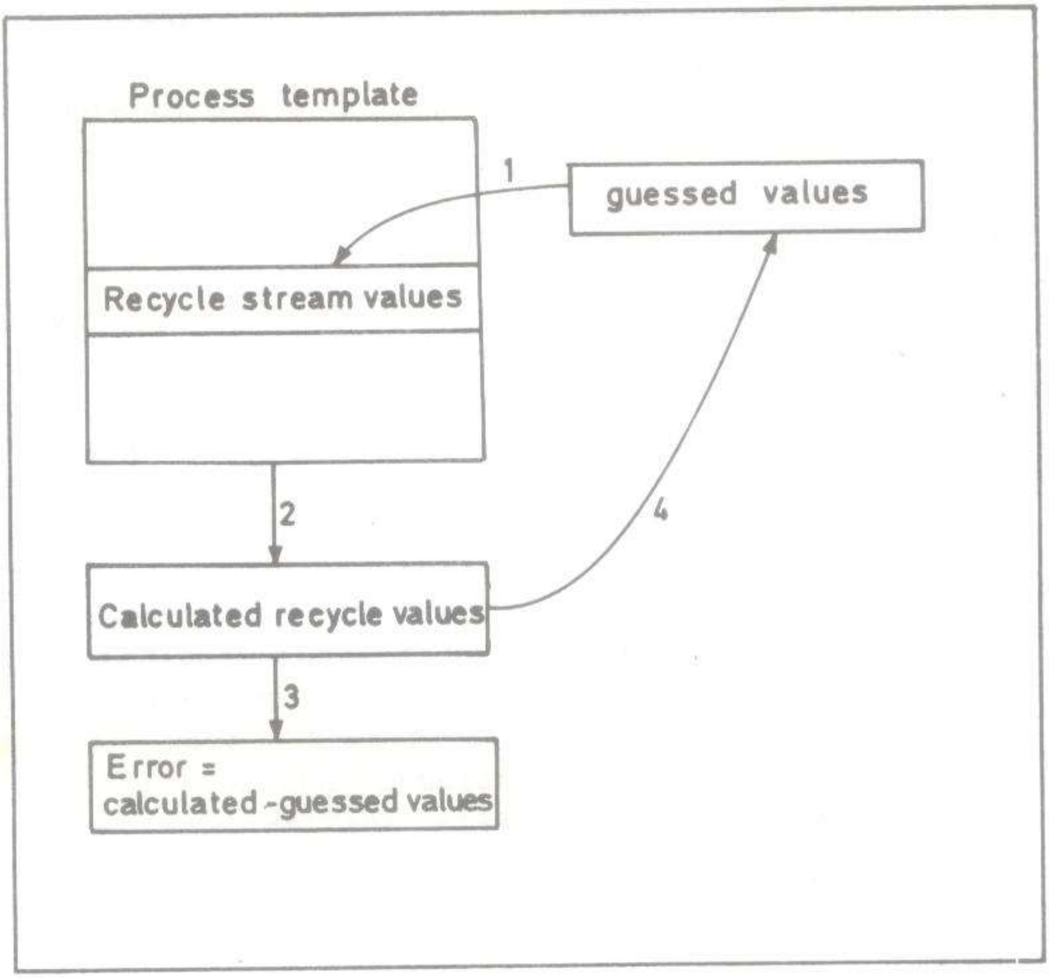
Two major approaches are available for flowsheet simulations. In the first approach, the sequential modular approach, the equations and constraints for each process unit are collected into separate computational subroutines or modules as well as solution procedures for the equations. Each Module would calculate values of the output streams for the given input conditions and the parameters for that unit, irrespective of the source of the input information or the sink of the output information. If the flowsheet contains a recycle stream, this approach require that the recycle stream be used in an iterative calculation at the flowsheet level. If **X** is set as the estimated recycle values of all variable in the tear stream, and f(X) as the calculated recycle values of all variable in the tear stream, then convergence is achieved when **f(X) = X** within a preset tolerance. Convergence promotion routines, such as the direct substitution and Bounded Wegstein methods are available to reduce the computation times required in the calculations.

In the second approach the equation oriented approach, the mathematical model of the process is organized and handled as one global set of equations representing the entire process, with any number of constraints which are added as equations to the overall set defining the problem. The equations are then solved simultaneously to give any values of output as required.

When the spreadsheet program is used for flowsheet simulation, the sequential modular approach can be applied. The formulae representing the unit process models are entered into the spreadsheet's template such that the output values of the units are calculated from the input values and unit parameters. Since the calculations are executed in column-wise or row-wise order, the modular representation of calculations would require that the formulae representing the recycle stream depend on values of variables which have not yet been calculated.

In order to calculate values of the variables in the recycle stream, the initial guesses of the torn stream, **X**, are entered to give values of the first iteration. This iterative procedure is continued by successively using the calculated values as the next guesses, such that new estimates of **X** are the most recently calculated values of **f(X)**. This sequence of calculation is demonstrated in Figure 1. Convergence is obtained when $X^{(r+1)} = X^{(r)}$ within present tolerance. Superscript **r** denotes r^{th} iteration.

The Use of spreadsheet program for flowsheet calculations including recycle calculations has been demonstrated by Julian (1985). Ferral et al.(1986) have used the spreadsheet for process analysis. In this work, the "ASEASYAS" spreadsheet program was used. In this program, a single worksheet consists of 1024 rows and 256 columns giving a total of 262144 uniquely defined cells with 480K memory. The program is Menu - driven and therefore is extremely easy to use. This program also has integrated graphics capabilities and can therefore be used to produce report - quality tables and graphs. **MACROS** can be used to provide Program - like functions. In this work, for example, MACROS were used to automatically copy the calculated recycle values into the guessed stream values for the next iteration. In this way once the initial guessed values are entered, the entire calculations proceed automatically once the programmed key is pressed.



Step 1 Input guess values

.. 2 Calculate flowsheet to get new values

.. 3 Calculate error, if required tolerance is not achieved go to step 4

.. 4 Copy calculated values into guessed stream values and repeat

Figure: 1 Sequence of calculations for flowsheet with recycle.

PROPOSED FLOWSHEET MODELS

The proposed oilseed processes must utilize solvents that can be produced locally, preferably from renewable agricultural resources. These solvents are mainly those that can be produced by processes of fermentation. Two main production routes are known in the manufacture of industrial solvents by microorganisms. The aerobic fermentation using yeasts to produce ethanol is a well established process. Anaerobic fermentation process such as that due to Weizman and Hamlyn (1920), produces a mixed solution containing acetone, butanol and ethanol, in varying concentrations depending on the type of microorganism used and the operating conditions.

Hron et al. (1984) have reported that alcohol-based solvents can be used in oilseed extraction. These reports also suggest that alternative solvent recovery methods, such as by cooling and phase separation can be employed instead of the energy-intensive distillation methods used in conventional hexane-based solvents can be used in oilseed extraction. These reports also suggest that alternative solvent recovery methods, such as by cooling and phase separation can be employed instead of the energy-intensive distillation methods used in conventional hexane-based processes. These reports further indicate that the by-products obtained after the extraction of oil have improved nutritional qualities. The following five cases were therefore selected for this investigation. The details of the formulation of the case studies is presented elsewhere, see Halfani (1988). The conventional process using hexane is included for comparative purposes.

Case 1 :This is the case of conventional processes using distillation method for solvent recovery

Case 2 :As in case 1 but, using 95% aqueous ethanol as solvent.

Case 3 :As in case 1, but using Acetone/Butanol/Ethanol (A/B/E) mixture as solvent.

Case 4 :This is the case of alternative solvent recovery by cooling and phase separation for oil/solvent mixture concentration using 95% aqueous ethanol as solvent.

Case 5 :As in Case 4, but using A/B/E mixture as solvent

Figure 2 shows the generalized flowsheet representing the five case studies.

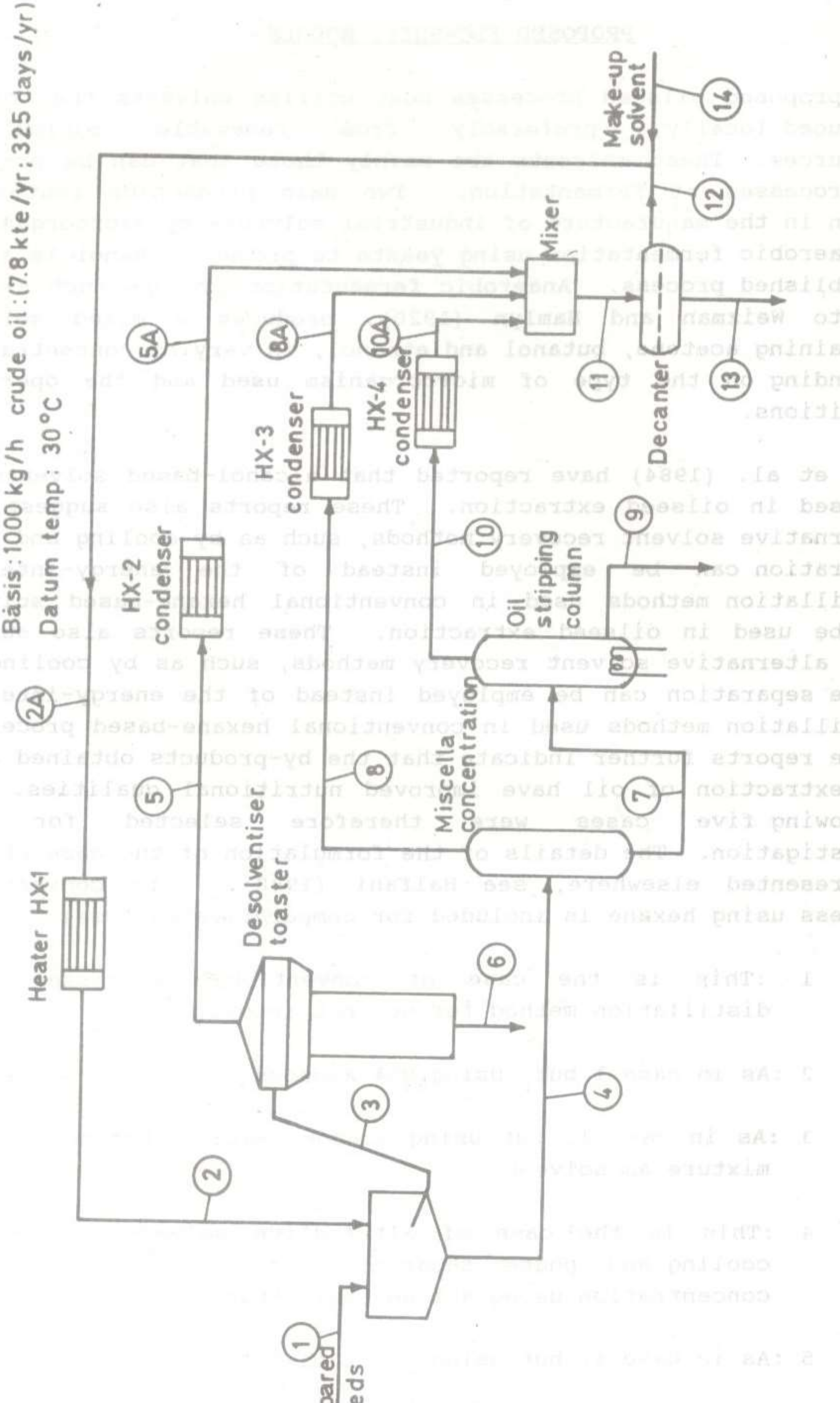


Figure: 2 General flowsheet for case studies

UNIT COMPUTATIONS

From the flowsheet of Figure 2, all process units can be represented by one or a combination of the elementary modules which involve mixing of a number of process streams, and/or separating a process stream into a number of output streams. The MIXER module; as represented in Figure 3a, is a device which accepts several inputs streams and aggregates them into a single output stream. The component balance equations for the MIXER will be given by equation [1].

$$F_S^{out} = \sum_{i=1}^{i} F_i \qquad S = 1, \ldots S \tag{1}$$

where the sum is over all input stream i.

The component separator is a device which will separate a feed stream into two or more output streams, as shown in Figure 3b. If there are J output streams, then the component balance equation is given by equation [2]

$$F_S^{in} = \sum_{i=1}^{i} F_i^J \qquad S = 1, \ldots S \tag{2}$$

The split fraction of component S is stream J is defined by the ratio

$$\alpha_S^J = \frac{F_S^J}{F_S^{in}} \tag{3}$$

By specifying the split fractions as separator equipment parameters, the output variables can then be calculated from known input values. Using these elementary modules, the modular representation of the flowsheet shown in Figure 2, is given in Figure 4.

DATA USED IN THE CALCULATIONS

For the flowsheet calculations, a large range of data input such as enthalpies, solute-solvent solubilities, heat transfer

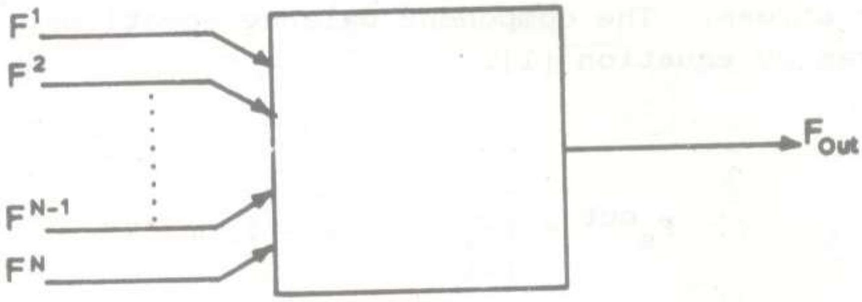


Figure 3.a Mixer module.

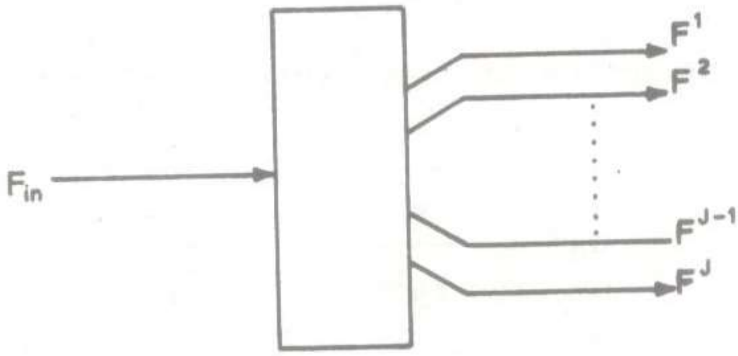


Figure 3.b Component separator

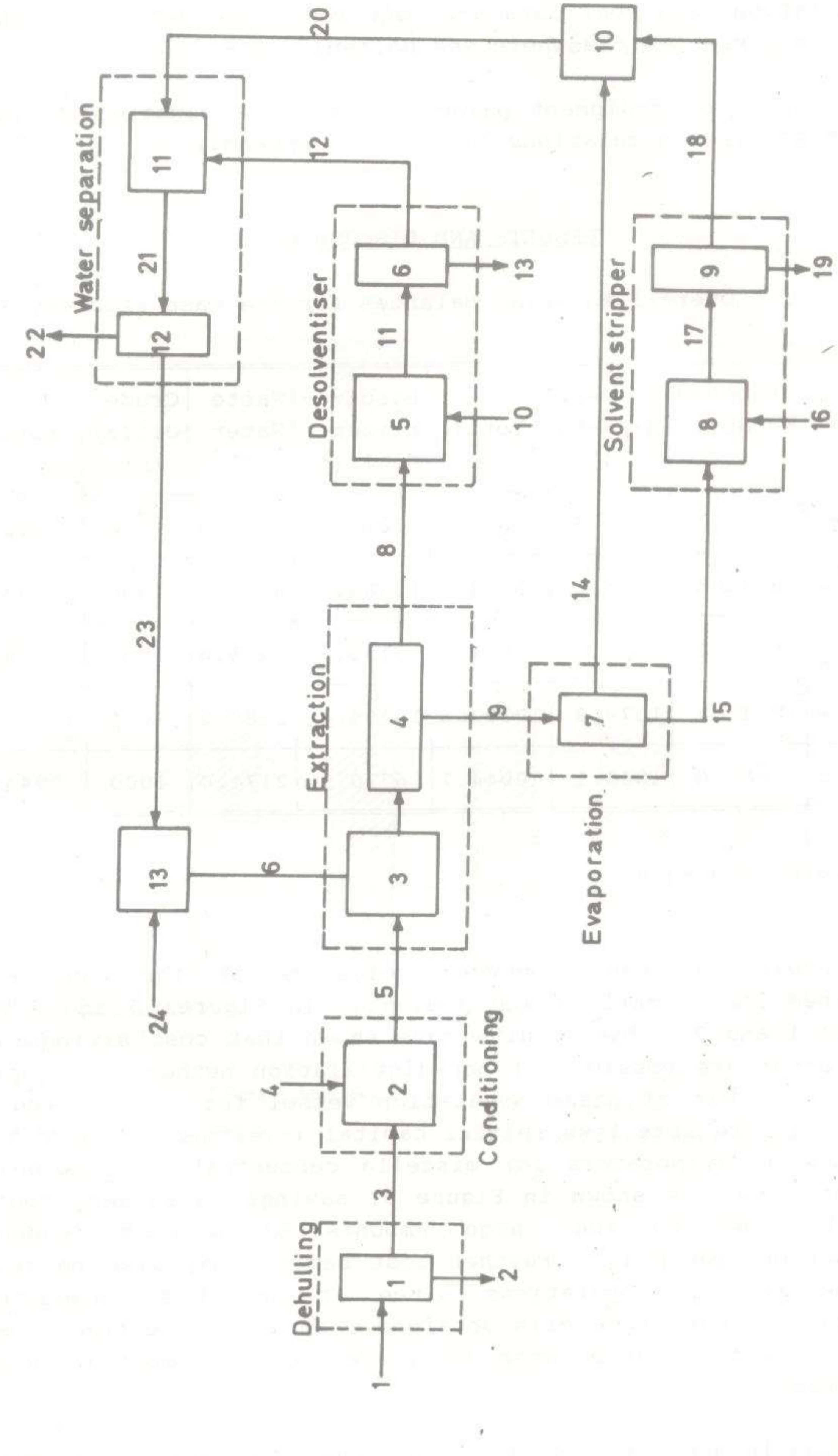


Figure 4 Modular representation of flowsheet of figure 2

coefficients, extraction rate data for the different solvent -seed combinations and cost data are required. The details of the data used is presented elsewhere see Halfani (1988)

The summary of equipment parameters and the constraints used for the Base Case calculations is given in Appendix 1.

RESULTS AND DISCUSSION

TABLE 1: Overall Material Balances for the Case studies.

Case	Prepared Seeds(1)	Solvent Make-up (14)	Total	Desolve-ntized Meal (6)	Waste Water (13)	Crude Oil(a) (9)	Total
Case1	4500.5	411.6	912.1	3087.5	824.6	1000	4912.1
Case2	13775.4	1055.6	15831.0	12483.9	2347.1	1000	15831
Case3	6763.0	811.9	7574.9	5155.5	1419.4	1000	1574.9
Case4	18113.7	1079.9	19193.6	15304.4	2889.2	1000	19193.3
Case5	8881.0	1063.1	9944.1	6770.1	2174.0	1000	9944.1

All values in kg/h

The results of the converged solutions of the case studies obtained are summarized and presented in Figures 5 and 6 and in Tables 1 and 2. The results have shown that cost savings in two main areas are possible if non-distillation methods are employed. First, the use of phase separation vessel for cooling and phase separation require less initial capital investment (Figure 5) than the use of evaporators for miscella concentration. Second, for ethanol case, as shown in Figure 6, savings in solvent costs are possible, despite the large amounts of solvent needed for extraction (Table 1). Further cost savings may also be realized in the refining operations since it has been suggested in literature that crude oils obtained from alcohol extractions have lower free fatty acids when oil is recovered by separation of the two phase.

Although it has been shown above that the use of alternative solvents has great potential, there are several limitations.

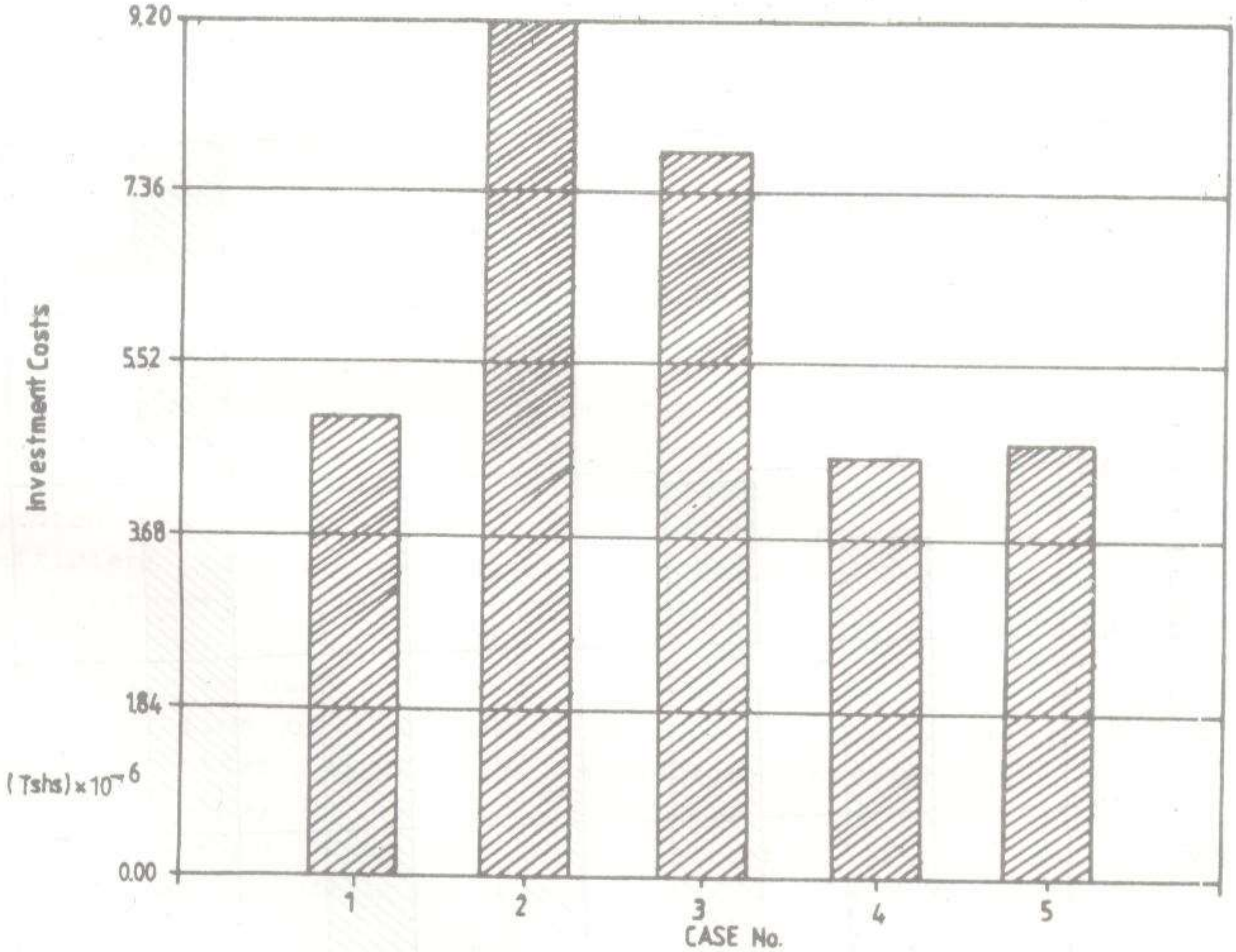


Figure: 5 Investment Costs for Solvent Recovery

Basic 7.8 kte crude oil/yr 325 days/y

1 kte = 10^3 tonne

All Costs at Dec 1989

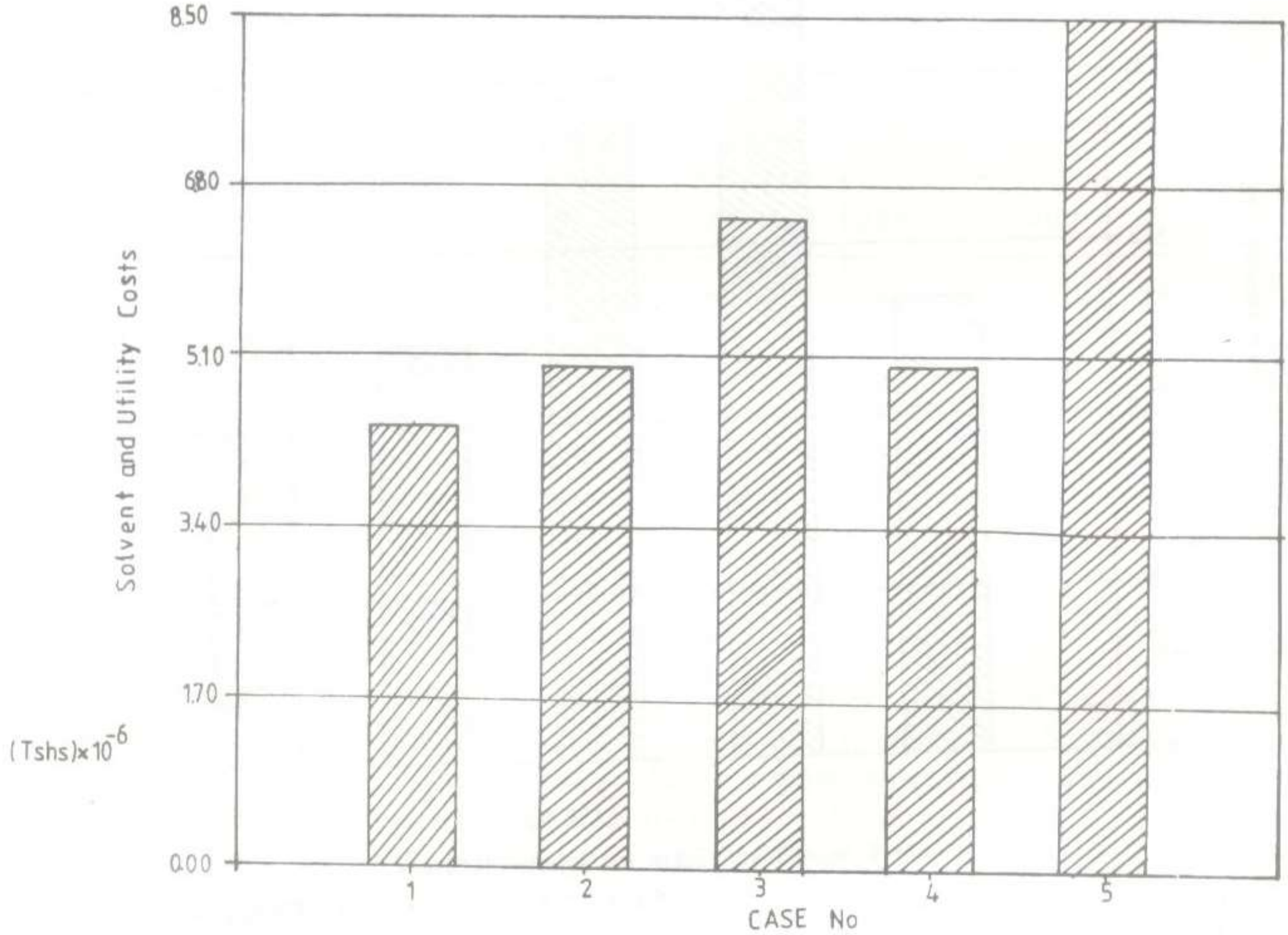


Fig:6 Solvent and Utility Costs Results
Besic: 78 kte crude oil/yr 325 days/y

1kte = 10^3 tone

All costs at Dec 1989

TABLE 2: Variation of Annual Utility Cost and Solvent Heating and Recovery Equipment cost using Sensitivity Analysis for Case 4.

Case	Annual Utility Cost (m.Tshs.)	Variation from Base	Equipment Cost (m.Tshs.)	Variation from Base
Base	887	-	4.38	-
-30% on Extraction Temp	828	+ 70%	5.58	+27%
-20% on phase separator parameter	1,516	+212%	6.6	+50%

Sensitivity results shown in Table 2 have revealed that in non - distillation cases, the variations in temperature during processing, especially in the phase separation vessel, can have a profound effect in the economics of the plant. Therefore the efficient operation will require careful control of temperature in both extraction and solvent recovery stages. Yet another disadvantage is that although it has been suggested that gravity separation be used to recover concentrated miscella, in practice the separation of the phases may not be easily attainable and therefore other alternative mechanical separations, such as centrifuges may be necessary. Further research is underway to investigate the phase separation characteristics of oil/alcohol and oil/alcohol/acetone mixtures.

Comparison of ethanol and A/B/E solvents in extraction using non - distillation methods (case 4 and 5) has shown that ethanol compare favorably with hexane conventional process (Case 1). Despite the lower solvent requirement for A/B/E/ (see Table 1), the higher costs for this solvent makes this alternative less favorable as compared to ethanol (Fig. 6).

CONCLUSIONS

The above investigation has highlighted two major areas which have to be considered when new processes for oilseed extraction are considered in Tanzania. First, it has been shown that the use of alcohol based solvents such as ethanol and acetone/butanol/ethanol mixtures should offer considerable investment savings if non-distillation methods of oil/solvent recovery methods are employed. A further economic benefit might be derived from the use of the oilseed cake and the refining of the oil products. Second, although it has been indicated that the use of alternative solvents has great potential, the efficiency operation will require careful control of temperature in both extraction and solvent recovery stages.

The preceding offers an example on how flowsheet calculations can be modelled using the spreadsheet program. This approach has several advantages:-

. The program is simple to use.

. It is cheap, and in most cases available in Public Domain Softwares at a very nominal fee.

. It is very flexible, therefore modifications in process model calculations can be easily made.

Although the spreadsheet program is simple to use, proper problem formulation must be exercised to avoid errors that may arise when inserting or deleting rows and columns. Convergence is easily achieved even when wild guesses are used. The spreadsheet, however, has limitations. ALL MENUs should be used with extreme care to ensure that the program is performing as expected by the user. However, since the spreadsheet is recalculated automatically as soon as a value or formula is changed, a wide range of possibilities can easily investigated. These are then used to select a few near - optimum flowsheets for further detailed study.

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APPENDIX 1

EQUIPMENT PARAMETERS AND CONSTRAINTS.

The following is a summary of equipment parameters used for the base case calculations.

Extractor
- residence time equivalent to t = 9 minutes for the laboratory extraction time t
- final miscella concentration is 20% for hexane at 60°C, and 12% for alcohols at 75°C.
- no solids in miscella
- total solvent hold-up in meal is 30% by weight.

Desolventiser toaster
- 90% of solvent in the extracted flakes is evaporated.

Evaporator
- final miscella concentration is 90%

Oil stripping column
- all oil recovered as crude oil
- 99% of solvent is recovered

Phase equilibrium separator
- outlet phases are in equilibrium
- residence time is one hour

Decanter
- 90% of solvent recovered
- all gums in alcohol phase removed for case 4 and 5.

Make-up solvent is 10% of recycle stream.

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