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FLOSHEET: Microcomputerized Flowsheeting/Simulation Program for Simulating Hydrogen Isotope Separation Processes

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ABSTRACT

Ontario Hydro has developed a comprehensive computer program, FLOSHEET, to simulate various hydrogen isotope separation processes, including water distillation and cryogenic distillation of elemental hydrogen isotopes. FLOSHEET was developed to assist in the operation and optimization of a Tritium Removal Facility Ontario Hydro is building at the Darlington Nuclear Generating Station. However, FLOSHEET is a general purpose simulator and allows the specification and simulation of complete process plants with various interconnected units. This paper discusses the development and features of FLOSHEET, as well as various simulation results which have emerged from the use of the program.

INTRODUCTION

Ontario Hydro has developed a process simulation and flowsheeting program, called FLOSHEET, which utilizes an IBM PC or compatible microcomputer to simulate various hydrogen isotope separation processes. This paper describes the development and features of the in-house program, and the applications that have proven its usefulness as a practical and cost-effective engineering tool.

Although it is a generalized flowsheeting program, FLOSHEET was primarily developed to assist in the commissioning and optimal operation of a Tritium Removal Facility (TRF), which is presently under construction at Ontario Hydro's Darlington Nuclear Generating Station. The TRF will extract tritium, a radioactive isotope of hydrogen, from the heavy water moderator of Ontario Hydro's CANDU nuclear reactors. This, in turn, will reduce radiological exposure of operating personnel and the public, and will facilitate maintenance by reducing tritium concentrations in the moderator systems. The TRF is scheduled for start up in 1987 and will produce tritium gas (T_2, atomic purity 99.9 percent), which will be immobilized in solid form as a metal hydride and stored or sold to commercial users. It will be the largest commercial hydrogen (H) - deuterium (D) - tritium (T) separation plant in the world.

The tritium removal process is composed of two inter-linked process units as shown in Figure 1. In the front-end unit, tritium is transferred from heavy water vapour into a circulating deuterium gas stream by equilibration over a platinum catalyst at 200°C, according to the reaction:

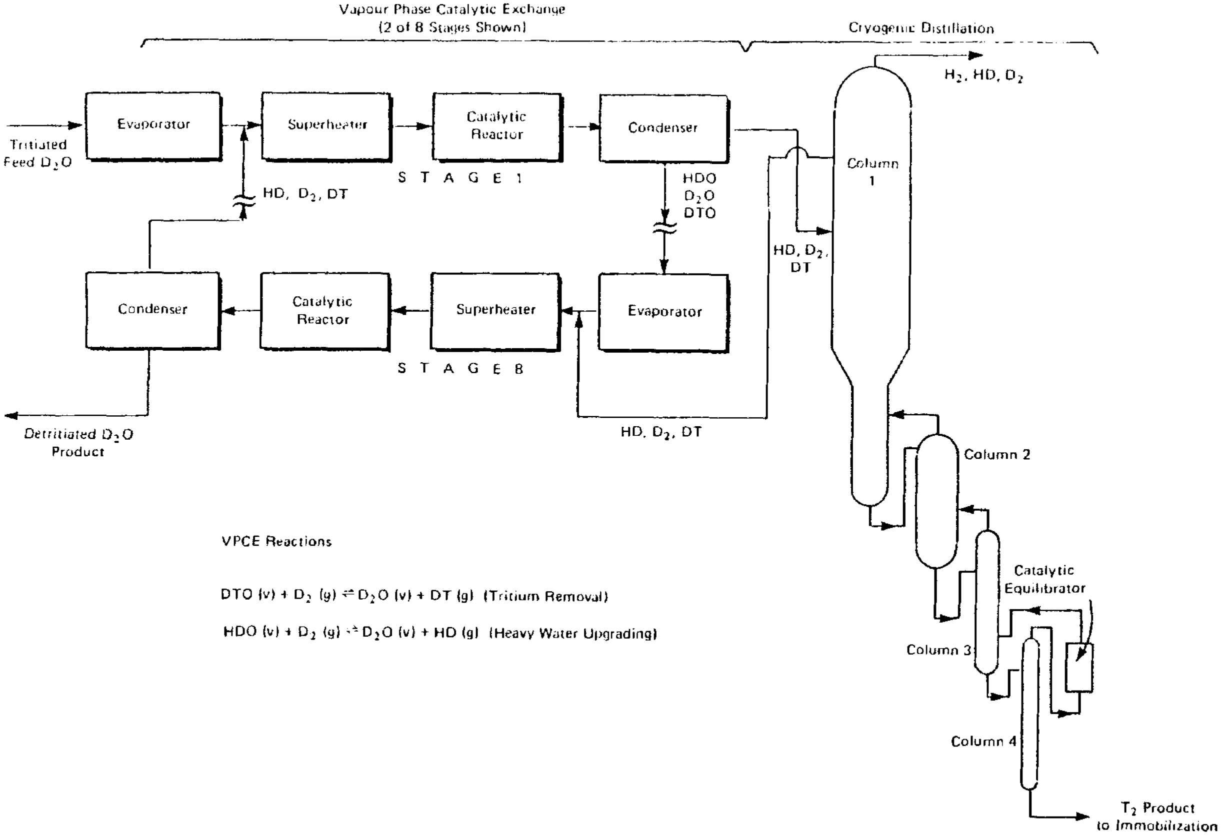
$$DTO + D_2 \rightleftharpoons DT + D_2O$$

The tritiated deuterium gas is then dried and cooled to 24K so that it will liquify under a reasonable pressure and permit the use of distillation. Separation of tritium from deuterium is performed in a series of distillation columns with several hundred theoretical stages and a catalytic equilibrator. The tritium is enriched from parts per million levels to the specified product concentration.

REASONS FOR DEVELOPING FLOSHEET

Computer simulation and flowsheeting is an established, cost-effective tool which allows process engineers to design and rate unit operations, processes, and entire process plants. In general, the benefits that accrue from process simulation include:

- Capital savings through improved designs.
- Decreased process engineering time spent on routine calculations, resulting in engineering manpower savings.
- Consistent and accurate data and techniques used throughout.
- Improved and quicker communication between design and operations staff.
- Improved troubleshooting and diagnostic capability.
- Faster commissioning and increased plant efficiency due to a better understanding of the limitations and flexibility of the process variables in the plant.



VPCE Reactions

$DTO\ (v) + D_2\ (g) \rightleftharpoons D_2O\ (v) + DT\ (g)$ (Tritium Removal)

$HDO\ (v) + D_2\ (g) \rightleftharpoons D_2O\ (v) + HD\ (g)$ (Heavy Water Upgrading)

FIGURE 1
Darlington Tritium Removal Facility
Process Flow Diagram

In addition to the above benefits, there are those that specifically result from the flowsheeting feature. These include:

* Elimination of the need for users to know complex mathematical and process engineering techniques such as convergence methods, matrix operations, etc.

* Availability of a consistent user interface, which promotes faster learning by new users, greater use by existing users, and continuity through staff turnover.

* Ability to easily incorporate process hardware modifications into the computerized simulation, without the need to modify the source code.

FLOSHEET was developed to enable examination of the impact of changing design and operating variables on the desired results of a process. Variables such as temperature, pressure, flow rate, stream composition, equipment characteristics and flow schemes can be assessed prior to building or commissioning a process plant. The benefits of doing this include being able to optimize the process, thus minimizing capital and operating costs.

For support of TRF operation, FLOSHEET will have a number of potential uses. It will enable parametric studies to be performed to produce "maps" which plot the impact of operating variables against TRF performance. It will be used for benchmarking the plant during commissioning. It will enable monitoring of TRF performance over time and will be used as a tool for diagnosing causes of operating problems.

FLOSHEET will also be used to gauge the effect of individual hardware or flow scheme changes. It will be used to examine the downstream effects of unavailability or removal/addition of a compressor or any number of VPCE stages from/to the front-end process. Similarly, the effects of various changes within the cryogenic distillation process will be assessed.

FLOSHEET - PROGRAM DESCRIPTION

Figure 2 outlines the various FLOSHEET components and how they interact. The program is comprised of:

(1) User Interface

(2) FLOSHEET Executive Program

(3) Unit Operations Models including:
    (a) VPCE/LPCE Front-End Process
    (b) Multicomponent Distillation
    (c) Catalytic Equilibrator

(4) Component Physical/Thermodynamic Property Library

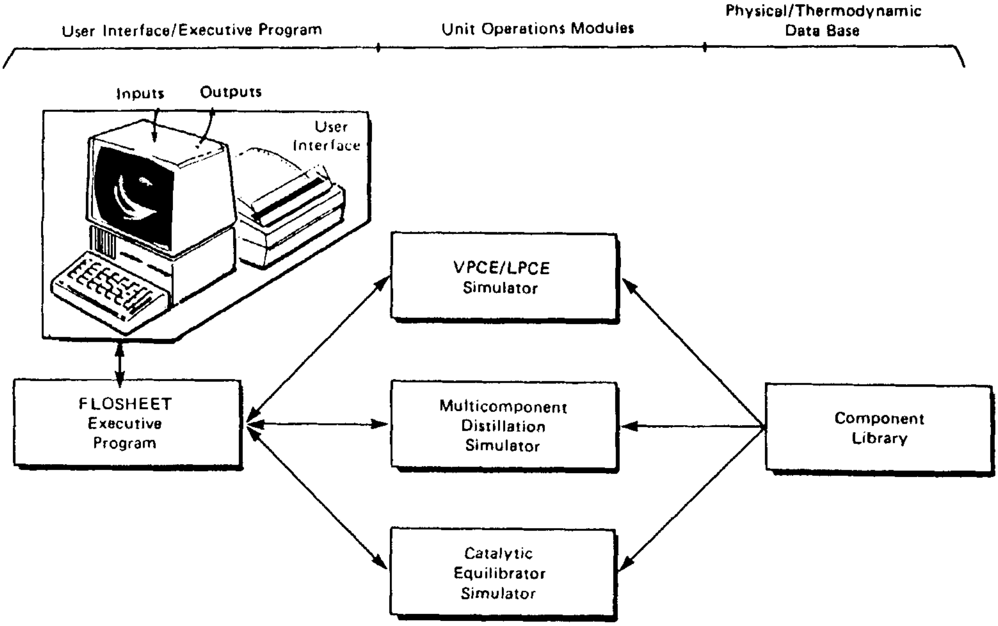


FIGURE 2
FLOSHEET Program Structure

Various arrangements of unit operations, including recycle streams, can be easily configured for simulation. All that is required to be input is the topology and the process variables for each stream/unit operation.

FLOSHEET can be extended to accommodate additional unit operations, a more comprehensive component library, or more comprehensive physical/thermodynamic data for each species. However, for applications envisioned at this time, the program is complete.

For the types of simulations being run, the only limitation is the computer time required. Presently, a single simulation run of the TRF takes approximately 10 minutes. This, however, is not felt to be a major drawback given the negligible cost per run.

User Interface

Input/output operations are simple, and utilize the typical hardware and software options available on microcomputer work stations. Input requirements are handled by constructing a file, not unlike those required for commercial simulation programs, using any text editor. The file is read by FLOSHEET and input data is checked. Input errors cause the program to terminate and provide appropriate diagnostic feedback. If the input file is correct in format and logically consistent, program execution proceeds.

During the simulation, intermediate convergence results of iterations within a distillation unit and for recycle loops in the process are echoed to the CRT monitor or a printer. The user can interrupt the run at any time if it is obvious that convergence is slow or not being achieved. The default option interrupts the simulation after a specified number of iterations, and alerts the user as to where convergence was not reached.

Considerable flexibility is available in obtaining a printout of exactly those results that are required. For both converged and unconverged results, the user can select, either a priori or upon completion of the simulation, any degree of output ranging from basic stream information to stage-by-stage results for the distillation column(s) and the VPCE/LPCE process.

Executive Program

The FLOSHEET executive program orchestrates the overall flowsheet simulation. FLOSHEET solves a specified process and provides for convergence of all inter-unit stream characteristics. These include temperature, flow, concentration, and pressure. Streams can be either liquid or vapour or liquid/vapour. Stream splitters or mixers are provided to facilitate flowsheeting.

The flowsheeting program has a sequential modular architecture. This was chosen because of its proven effectiveness and its acceptance by major flowsheeting systems such as ASPEN and PROCESS^{sm}, and by most in-house industrial simulators (2).

The recycle and unit computational sequences are determined automatically or can be specified by the user. Recycle convergence is accelerated by the bounded secant method (3), which we have found to be reliable and which generally provides rapid convergence of recycle stream values.

FLOSHEET is both rigorous and expandable. Not only does it provide effective convergence for all recycle streams in a given flowsheet, but there is no practical limit to the number or kind of recycle configurations that can be solved. Multiple stream nesting arrangements or stream crosses, such as those shown in Figure 3 can be handled without difficulty by the program. The design of the executive program also allows for the addition of any number of unit operations, components or property data. As long as a standard interface format for additions is adhered to, the modular nature of Ada allows a programmer to independently add unit operation models or construct component/property libraries for incorporation into FLOSHEET.

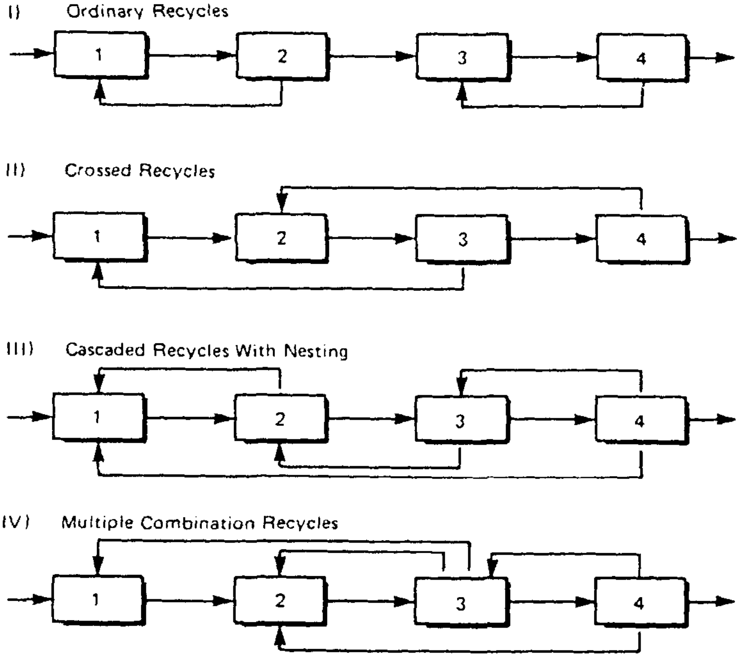


FIGURE 3
Typical Recycle Problems
Solvable with FLOSHEET

The design of the FLOSHEET executive program uses a new recursive technique made possible by use of the Ada language (recursion is also possible with languages such as Pascal and C) for determining sequences of unit computations and treatment of recycle streams. This method of solution would not be possible using a non-recursive language such as FORTRAN. The heart of the algorithm is a procedure for solving a general unit by calling the appropriate unit operations routine. However, a unit can only be solved for if all input streams are known. If some input streams are not known, this means that an upstream unit needs to be solved for before the calculation can proceed. Thus, the procedure calls itself to solve the upstream unit(s) before returning to solve the one at hand. This type of walk back recursion continues until a unit with all input streams known is found and solved for, and then the procedure walks forward to solve the unit at hand.

In the case of recycle streams, the algorithm will walk back until it encounters the original unit. In this case identified recycle streams are tagged as known and stream estimates (usually supplied by the user) are used for calculate the unit and then the procedure returns back around the recycle loop. The recycle loop is iterated until all recycle streams converge.

The virtue of using a recursive technique for solving a network of interconnected units is that the code for the executive program is very compact (less than 500 lines), easy to program, and conceptually easy to understand.

Traditional flowsheeting executive program algorithms written in FORTRAN and very cumbersome in comparison and involve many thousands of lines of code.

Unit Operations

VPCE/LPCE† front-end process. The VPCE/LPCE model is shown in Figure 4. The simulation program has a number of features, which include:

- Simulation of any number of VPCE or LPCE stages.
- Solution of both upgrading and tritium removal reactions simultaneously.
- Ability to vary reaction temperatures, gas and liquid flow rates, and inlet stream concentrations.

An individual run for an eight-stage VPCE, which simulates the TRF, requires only a few seconds.

Multicomponent distillation. The rigorous multicomponent distillation model is shown in Figure 5. It is the most complex unit operation in the TRF. The features of the distillation model include:

- Capability to model water distillation based heavy water upgrading or cryogenic distillation of gaseous hydrogen isotopes.
- Material and energy balances for each stage.
- Incorporation of liquid and gas phase non-idealities. The effect of the temperature dependence of the non-idealities

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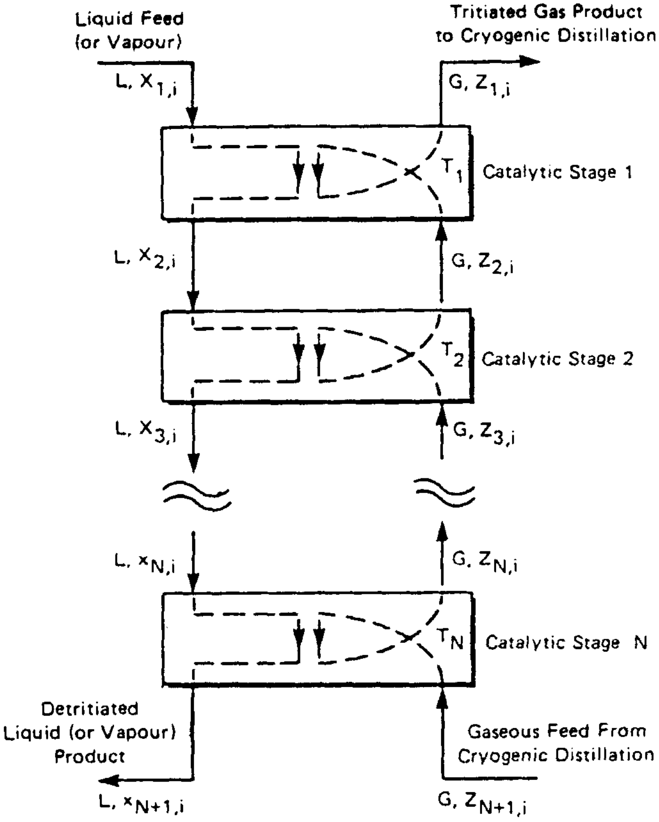
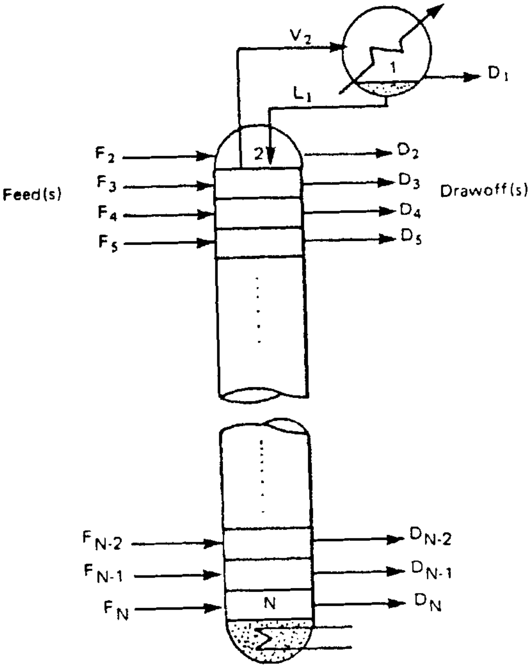
†LPCE or Liquid Phase Catalytic Exchange, is almost identical to VPCE, except that the catalysis involves a liquid/gas reaction rather than vapour/gas. The differences in the processes (i.e., catalyst, operating temperature, cooling and heating loads) are not a limitation on the simulation model.



Primary Reactions: $D_2 + DTO \rightleftharpoons DT + D_2O$ (Tritium Removal)

$D_2 + HDO \rightleftharpoons HD + D_2O$ (Upgrading)

FIGURE 4
VPCE/LPCE Model



Overall Model

Single Stage Model

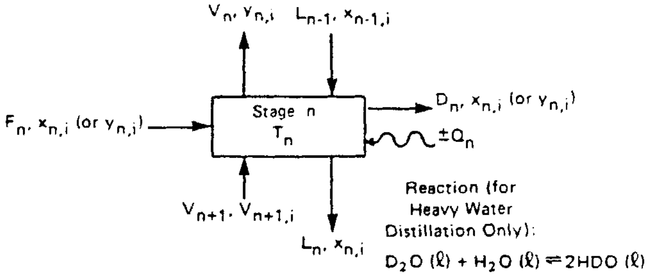


FIGURE 5
Cryogenic Distillation Model

is also incorporated. This is important because over many stages of separation, the importance of non-idealities and their temperature dependence is magnified.

- Rigorous stagewise calculations performed for up to a 1000 (theoretical) stage column.
- Heat input/removal can be simulated on any stage. This is particularly important for simulating radioactive decay heat from concentrated tritium in the final column.
- For the simulation of water distillation for heavy water upgrading, the liquid phase equilibration reaction between H_2O, HDO, and D_2O is incorporated into each stage. This is an important consideration as the reaction plays a major role in the distribution of the H, D, and T isotopes throughout the column.

The distillation column algorithm used by FLOSHEET is specifically designed to overcome problems which are encountered in the simulation of isotope separation distillation columns. Isotopic distillation typically involves column with a large number of theoretical plates and very high degrees of separation. Both these factors contribute to difficulties with traditional distillation column algorithms such as the equation decoupling - relaxation methods of Thiele-Geddes (1) or Holland (4) and the linearization methods of Napthali-Sandholm (5), Tomich (6) or Kinoshita (7). The equation decoupling-relaxation methods become unstable and experience convergence difficulties when the number of stages or number of components become large, and when non-ideal mixtures are encountered. The linearization methods generally converge, if a reasonable starting guess can be made to begin the iteration, however, these algorithms exhibit dramatic increases in computation time and storage requirements because of large Jacobian matrices, when the number of theoretical plates becomes large. For 700 theoretical plate heavy water distillation columns, these methods are impractical. (It is interesting to note, however, that recently Kinoshita (8) has proposed a Newton-Raphson method for heavy water distillation columns in which the Jacobian matrix is block-tridiagonal, resulting in relatively low storage requirements and fast execution times. This method appears to be promising for these types of calculations.)

The distillation column algorithm used by FLOSHEET is briefly described below. For clarity, the algorithm is described for the case of ideal solutions with no energy balances. Further details of the method, including incorporation of non-idealities and energy balances will be described in a later paper.

The species mass balance equations for a distillation column may be written as:

$$\underset{\sim}{A}_i \, \underset{\sim}{x}_i = \underset{\sim}{f}_i \quad , \; i = 1, \ldots, \text{Number of Components} \qquad (1)$$

The matrix $\underset{\sim}{A}_i$ is tri-diagonal and a function of the liquid and vapour flow throughout the column, the feeds, drawoff rates and the species K values ($y_{n,i} = K_i(T_n)\, x_{n,i}$) where n is the plate and i is the species. For ideal solutions, the K values are strictly functions of temperature. The right-hand-side of equation (1) is a constant vector given by the column feed stream specifications.

A unique characteristic of isotopic distillation is that columns operate with very little temperature difference between the top and the bottom of the column. Thus, whatever the scheme for solving the column, from iteration to iteration, the temperature variation on any given plate of the column is exceedingly small. This feature allows linearization of the temperature dependence of the K values down the column as $K_{n,i} = \alpha_{n,i} + \beta_{n,i}T$. For each theoretical plate, the values of α and β can be computed (and recomputed if required between iterations) to accurately reflect the K value temperature dependencies for that plate. This decomposition of the K values allows equation (1) to be written as:

$$\underset{\sim}{B}_i\, \underset{\sim}{x}_i + \underset{\sim}{C}_i\, \underset{\sim}{T}\, \underset{\sim}{x}_i = \underset{\sim}{f}_i \tag{2}$$

where $\underset{\sim}{B}_i$ and $\underset{\sim}{C}_i$ are temperature independent square matrices, and $\underset{\sim}{T}$ is a diagonal matrix corresponding to the column temperature profile. Noting that x_i must sum to 1 for each stage, if a guess $\underset{\sim}{T}^o$ is made for the column temperature profile and $\underset{\sim}{T}^*$ is the desired solution, from equation (2), it can be deduced that $\underset{\sim}{T}^*$ is related to $\underset{\sim}{T}^\circ$ through the equation:

$$\underset{\sim}{T}^*\, \underset{\sim}{1} = \underset{\sim}{T}^\circ \sum_i \underset{\sim}{x}_i^\circ + \sum_i \underset{\sim}{C}_i^{-1}\, \underset{\sim}{B}_i\, [\underset{\sim}{x}_i^\circ - \underset{\sim}{x}_i^*] \tag{3}$$

Equation (3) is exact and involves no simplifying assumptions. However, it cannot be solved directly since $\underset{\sim}{x}_i^*$ are not known a priori. To be able to use this equation one can use the approximation that for each plate

$$x^*_{n,i} \approx \bar{x}_{n,i} = x^\circ_{n,i} / \sum_i x^\circ_{n,i} \tag{4}$$

This assumption leads to the recurrence relation between iteration r and r+1 of:

$$\underset{\sim}{T}^{r+1}\, \underset{\sim}{1} = \underset{\sim}{T}^r \sum_i \underset{\sim}{x}^r_i + \sum_i \underset{\sim}{C}^{-1}_i\, \underset{\sim}{B}_i\, [\underset{\sim}{x}^r_i - \bar{\underset{\sim}{x}}_i^r] \tag{5}$$

which is readily solved for once the matrix product ($\underset{\sim}{C}_i^{-1}\, \underset{\sim}{B}_i$) is pre-computed. It should be noted that the matrix product ($\underset{\sim}{C}_i^{-1}\, \underset{\sim}{B}_i$) is of dimension NxN, where N is the number of theoretical plates. However, this matrix is in fact rather sparse - with only two diagonals plus an additional column for each plate with a drawoff. This sparsity may be taken advantage of and results in low storage requirements and fast computation times. For typical high performance columns, the algorithm converges in 5 to 10 iterations. In contrast, hundreds of iterations may be required by equation decoupling-relaxation methods. Typical computation time for a 100 plate column separating six components is in the range of 10 seconds to 2 minutes on an IBM PC equipped with the 8087 math coprocessor.

Catalytic equilibrator. The equilibrator is required for the conversion of DT or HT to T_2, and is required in the DTRF to ensure that pure T_2 can be drawn off the bottom of the final column.

A representation of the catalytic equilibrator model, including the three simultaneous reactions involved, is provided in Figure 6.

Component Physical/Thermodynamic Property Library

A separate component library has been incorporated into the simulation model, which allows any unit operation to access various physical, chemical and thermodynamic properties. Presently, the library includes 12 components:

I. H_2, HD, HT, D_2, DT, T_2

II. H_2O, HDO, HTO, D_2O, DTO, T_2O

For the components of Group I, the properties that have been provided are:

- Pure component vapour pressures in the range 20-30 K.
- Vapour and liquid non-ideality data for mixtures in the range 20-30 K.
- Liquid and vapour enthalpies in the range 20-30 K.

For the components of Group II, the properties that have been provided are:

- Pure component vapour pressures in the range 0-300°C.
- Liquid and vapour enthalpies in the range 0-300°C.

SIMULATION RESULTS

As part of the development schedule, each of the unit operations was modelled and tested. Testing is continuing at this time, however each individual unit operation has been successfully benchmarked against either calculated results, or results from other proven computer models.

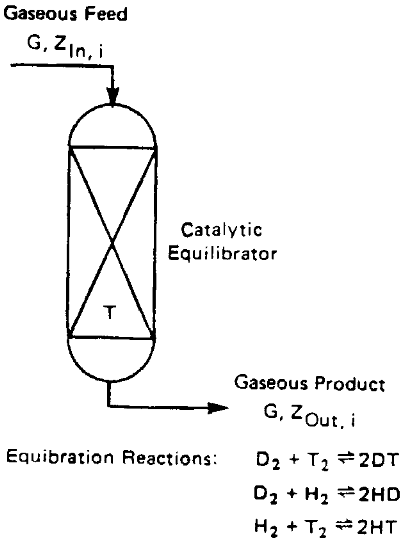


FIGURE 6
Catalytic Equilibration Model

Various results from FLOSHEET simulation are provided below.

VPCE Front-End Process

Simulation of the VPCE has been performed for a large number of cases. These cases address changes in operating variables that may be expected to actually occur within the front-end process. Two representative simulations are discussed below:

Combined temperature/number of stages effects on TRF performance. In Figure 7 the effect of changing either or both the (VPCE catalyst) temperature and the number of VPCE stages is shown. This figure represents a typical "map" that would be prepared for operation and commissioning support of the TRF. Numerous similar maps would enable operators to better understand the consequences of all expected process variable changes in the plant.

The effect on TRF capacity of temperature changes and number of stages in operation is seen to be minimal. The reduction in TRF capacity due to a loss of three VPCE stages and a reduction in catalyst temperature of 25% (50°C) is only 4%. This is, nonetheless, an important result, and indicates that these process variables do not have to be monitored as carefully as others.

There is an indication that using lower than 200°C temperatures may result in energy savings with only minimal effect on tritium removal performance. This saving may be exploited to the point where liquid carryover into the catalyst begins to poison it (approximately 100°C to 150°C).

From Figure 7 it can also be noted that TRF capacity can not be noticeably enhanced by increasing VPCE catalyst temperature. The tritium removal reaction's equilibrium constant is known to increase at higher temperatures, but a 50% (100°C) rise in catalyst temperature only increases the tritium removal capacity by a fraction of one percent. It is questionable whether the increased energy requirement could be justified by the marginal improvement in tritium removal capability.

Effects of the VPCE gas/liquid (G/L) ratio on TRF performance. Figures 8 and 9 show the results of various G/L ratios given a constant G or L, respectively.

Figure 8 shows that tritium removal capability is almost directly proportional to the liquid flow rate. For example, if the liquid flow rate is increased to 125% of its design value the tritium removal rate also increases to 121% of the design rate. Similarly, as the liquid flow rate is reduced, the tritium removal rate is also reduced.

On the other hand, Figure 9 shows that the tritium removal rate in the VPCE is not a function of the gas flow rate. Decreasing the gas flow through the VPCE to 80% of design reduces the tritium removal rate by only 4%.

The implication of Figures 8 and 9 is that there is some potential for optimizing tritium removal operations. The extent to which this may be done will be determined during the commissioning and early operation of the plant.

Multicomponent Distillation

The multicomponent distillation model can be used to simulate either the cryogenic distillation process in the TRF, or water distillation based heavy water upgrading. Results from both types of simulations are described briefly below.

Cryogenic distillation results. Figure 10 provides comparative results from three cryogenic distillation models. Using identical input data representative of hydrogen isotope distillation, the PROCESS simulator and two types of FLOSHEET simulations were compared as to their calculated product concentrations.

FLOSHEET results from using vapour pressures of pure components, provide an interesting comparison. Using ideal vapour pressures of pure components, results for both PROCESS and FLOSHEET are essentially identical.

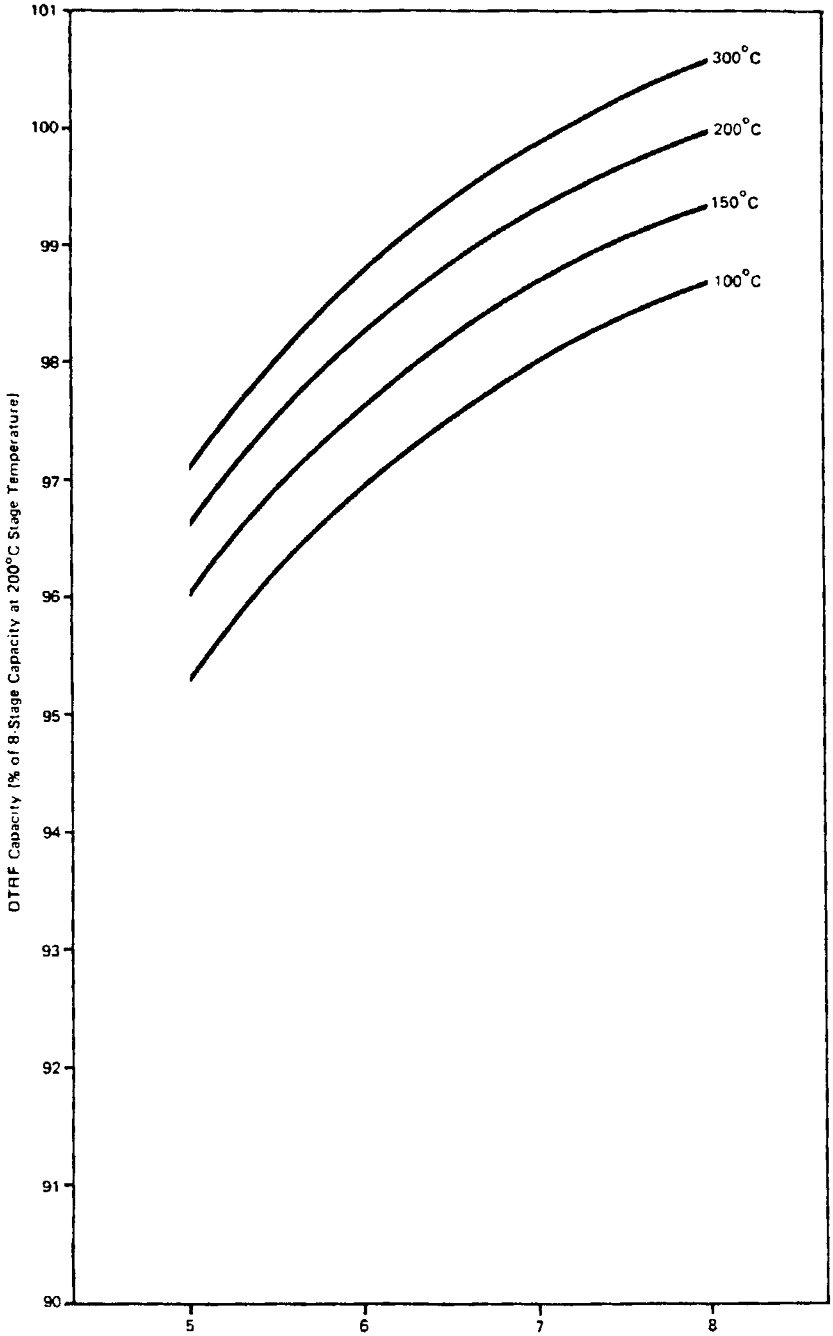
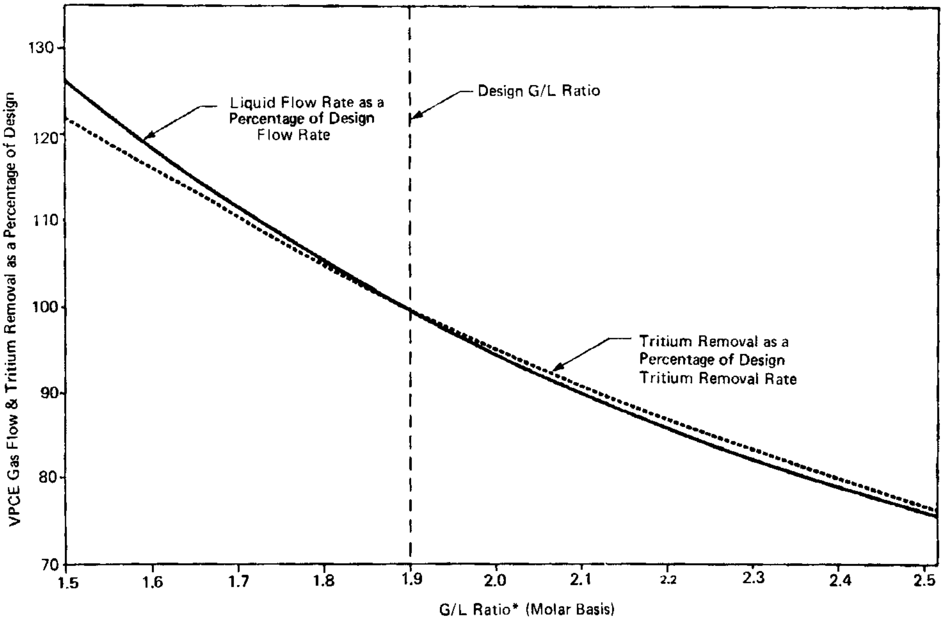


FIGURE 7
Combined Temperature/Stage Effects on DTRF Capacity



* G is assumed constant – L is varied

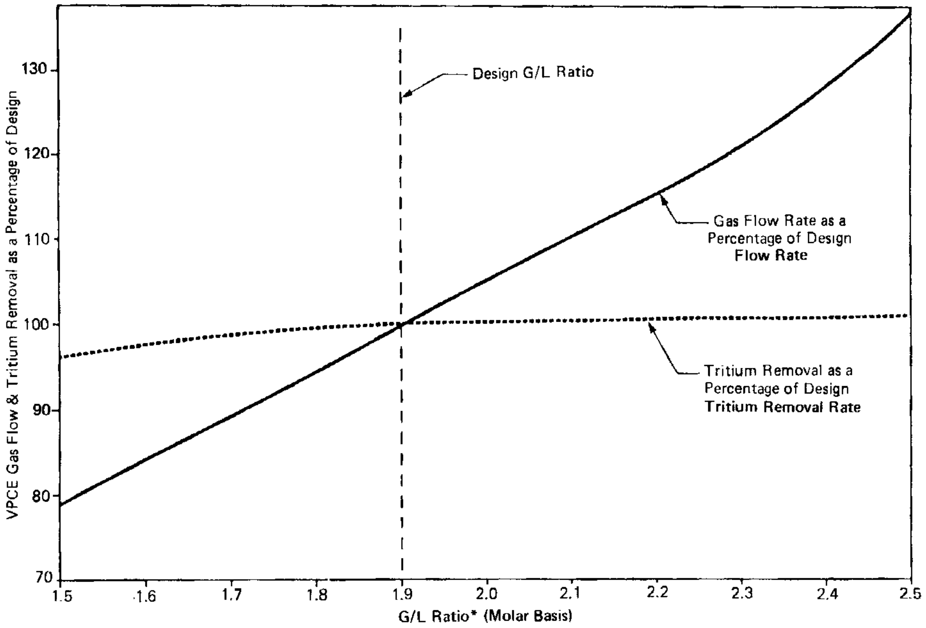
FIGURE 8
G/L Ratio Impact on DTRF Capacity – I

The second column in Figure 10 shows FLOSHEET distillation model results which incorporate the temperature dependency of non-idealities. These results are closest to those that will be experienced during operation.

The PROCESS simulator has the capability of incorporating non-idealities, however the temperature dependencies of the non-idealities are not incorporated due to the input limitations of the program. PROCESS results are shown in the third column in Figure 10.

A comparison of both top and bottom product results yields important differences. For the top product results, the difference in the HT component is significant and is the only one examined in detail here.

Both FLOSHEET and PROCESS (non-idealities models) yield HT concentrations several orders of magnitude greater than those using pure component vapour pressures.



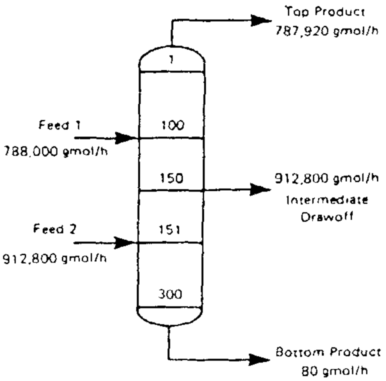
* L is assumed constant - G is varied

FIGURE 9
G/L Ratio Impact on DTRF Capacity – II

Of greater concern is the difference between the (non-idealities included) FLOSHEET and PROCESS models' predicted product concentrations of HT. Assuming complete removal of HT (i.e., HT top product concentration is zero) represents 100% removal, PROCESS predicts 99.7% removal for the existing column. FLOSHEET predicts a 94.2% removal, or 5.5% less than PROCESS. This constitutes a sizeable reduction in tritium removal capacity and is an important result that emerges from the more accurate calculations designed into FLOSHEET.

Heavy water upgrading results. Figure 11 shows a comparison of heavy water upgrading results using two different models available in FLOSHEET. The first column shows the results of a binary approximation (D_2/HD distillation) method. The results in the second column are more rigorous and include the three-component equilibrium reaction occurring on each stage. This distillation plus chemical reaction model provides a truer picture of the behaviour of heavy water distillation.

There are two significant results that can be noted from Figure 11. First, FLOSHEET provides concentration data on all three



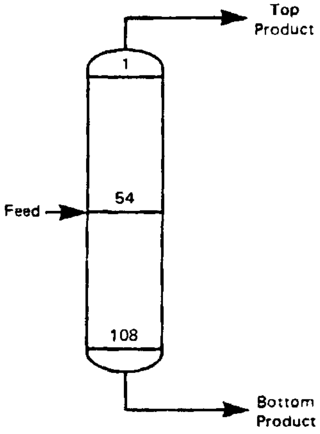
Feed Compositions	Feed 1	Feed 2
H_2	9.9972×10^{-1}	9.7814×10^{-1}
HD	2.6988×10^{-4}	2.0631×10^{-2}
HT	1.2494×10^{-5}	1.2310×10^{-3}
D_2	2.2354×10^{-8}	2.2001×10^{-6}
DT	2.2737×10^{-9}	2.4010×10^{-7}
T_2	6.0534×10^{-11}	5.9642×10^{-9}

Top Product Results

		Compositions (Mole Fractions)	
Component	FLOSHEET (Ideal K's)	FLOSHEET (Non-idealities)	PROCESS* (Non-idealities)
H_2	9.999×10^{-1}	9.998×10^{-1}	9.999×10^{-1}
HD	6.096×10^{-5}	1.113×10^{-4}	8.368×10^{-5}
HT	2.948×10^{-12}	7.261×10^{-7}	3.973×10^{-8}
D_2	2.267×10^{-25}	1.066×10^{-15}	4.950×10^{-19}
DT	2.397×10^{-37}	5.913×10^{-24}	8.585×10^{-27}
T_2	1.122×10^{-49}	2.179×10^{-33}	1.874×10^{-37}
		Bottom Product Results	
H_2	2.134×10^{-27}	2.300×10^{-26}	1.3987×10^{-18}
HD	8.669×10^{-1}	9.017×10^{-1}	8.9579×10^{-1}
HT	1.326×10^{-1}	9.801×10^{-2}	1.0391×10^{-1}
D_2	3.637×10^{-4}	2.524×10^{-4}	2.6844×10^{-4}
DT	5.394×10^{-5}	3.463×10^{-5}	3.5289×10^{-5}
T_2	1.991×10^{-6}	1.221×10^{-6}	1.2763×10^{-6}

* PROCESS results failed to converge. Unconverged results are shown.

FIGURE 10
Comparison of Column Simulation Results
For Hydrogen Isotope Distillation



Basic Column Data

Max. No. Iterations		=	50
Column Height	(m)	=	20.000
Column Diameter	(m)	=	1.880
Feed Position	(m)	=	10.000
Top Pressure	(kPa a)	=	13.000
Steam Usage	(kg/h)	=	7000.000
Steam Pressure	(kPa g)	=	250.000

Feed Stream

Temperature	(deg K)	=	325.0000
Liquid Feed Rate	(gmole/s)	=	5.0000

Liquid Mole Fractions
H_2O : 7.00000E-1
D_2O : 3.00000E-1

Product Drawoff Streams

1. Overhead
   Liquid Drawoff Rate, gmole/s = 3.55000 Vapour Drawoff Rate, gmole/s = 0.00000
2. Bottoms
   Liquid Drawoff Rate, gmole/s = 1.45000 Vapour Drawoff Rate, gmole/s = 0.00000

Top Product Results

Component	Compositions (Mole Fractions)	
	FLOSHEET (Binary Approx.)	FLOSHEET (Distillation + Rxn)
H_2O	8.861×10^{-1}	7.900×10^{-1}
HDO	N/A	1.971×10^{-1}
D_2O	1.139×10^{-1}	1.279×10^{-2}
	11.39 % D	11.13 % D
Bottom Product Results		
H_2O	2.444×10^{-1}	5.803×10^{-2}
HDO	N/A	3.603×10^{-1}
D_2O	7.556×10^{-1}	5.816×10^{-1}
	75.56 % D	76.18 % D

FIGURE 11
Comparison of Column Simulation Results
For Heavy Water Upgrading

components involved in the distillation. The binary approximation deals with the separation of only two components and lumps the third component in with the other two. The primary benefit of knowing the concentration of the three components is that it provides an accurate representation of the component concentrations in the liquid mixture at any point.

The second major difference is in the predicted deuterium concentrations (isotopics), in both top and bottom product streams. The FLOSHEET distillation plus reaction model predicts a lower isotopic mole fraction of deuterium in the top product and a higher isotopic in the bottom product than does the binary approximation model. For actual working columns, a one percentage point difference in bottom product isotopic mole fraction can mean the difference between usable reactor grade heavy water and non-reactor grade water. As the binary assumption model produces results that are too conservative, columns operated according to this model would not achieve their full capability. This would result in sub-optimal operating conditions and higher than necessary operating costs.

APPLICATIONS

Initially FLOSHEET was used only for design simulation of the TRF. Presently, extensive process simulations are being performed to assess key process design parameters for commissioning support, and to optimize operating modes and operating strategies. The program has also been adapted to simulate water distillation based heavy water upgrading plants. Ontario Hydro operates nine of these plants. In the future, it is expected that FLOSHEET will be installed locally as a standard operations support tool in both types of plants. This will mean continued use of the program by operations personnel for increasing plant yield and optimizing production.

Recognizing that there are numerous operators of water distillation plants, and several cryogenic distillation based hydrogen isotope separation installations, investigations are underway to determine the potential for a commercial version of FLOSHEET.

Other opportunities for the application of FLOSHEET have also emerged. Ontario Hydro has recently been involved in US and European design studies of thermonuclear fusion reactor fuel cycles (based on D2-DT fusion). These fuel cycles typically involve the purification, separation and concentration of gaseous H,D,T, combinations. FLOSHEET has been, and is continuing to be, used in fusion reactor fuel system design.

All of the above applications involve use of the present steady state FLOWSHEET simulator. In addition, we are currently considering dynamic process modelling to aid in the interpretation of non-steady state processes, such as the TRF batchwise T_2

product drawoff. As it can take up to several days of operation before on-spec tritium drawoff is possible from the TRF, prior knowledge of tritium concentration and inventory profiles at any time would enhance the ability to properly and efficiently schedule drawoffs. Also, because on-line sampling of the purity of the tritium product stream at the bottom of the final TRF column is not practical due to the complexities and hazards involved, dynamic computer simulation is the only way to accurately assess the drawoff concentrations at any given time.

SUMMARY

The development of FLOSHEET has provided design and operations support personnel in Ontario Hydro with a state-of-the-art tool for simulating various hydrogen isotope separation processes more accurately and more cost-effectively than previous in-house programs or a commercial simulator package.

Implemented on an IBM-PC or compatible microcomputer, FLOSHEET, nonetheless, has features similar to those of commercial simulation programs on main-frame computers. Simplicity and a consistent user interface, were major considerations in the development of the program. Technical characteristics include rigorous models of the unit operations, and easily supportable software that is flexible and expandable.

Originally developed for use as a simulator for the Darlington Tritium Removal Facility, FLOSHEET can simulate a number of hydrogen isotope separation processes and process variants. Presently, it is used in-house for the simulation of tritium removal processes, heavy water upgrading processes based on water distillation, and fusion fuel cycle subsystems. Minor modifications will allow the simulation of other isotope separation processes, such as carbon-14 distillation. Efforts are underway to develop the commercial potential of FLOSHEET and plans have also been made to develop a dynamic simulation version of FLOSHEET.

NOMENCLATURE

D_n - flow rate of distillation product stream from n'th stage

F_n - flow rate of distillation feed stream to n'th stage

G - flow rate of gaseous stream in VPCE/LPCE, catalytic equilibrator

L - flow rate of liquid (vapour) stream in VPCE/LPCE

L_n - flow rate of liquid stream leaving n'th stage

N - total number of theoretical stages

Q_n - heat input/removal on n'th stage

T_n - temperature on n'th stage

V_n - flow rate of vapour stream leaving n'th stage

$X_{n,i}$ - mole fraction of component i in liquid stream leaving n'th stage

$Y_{n,i}$ - mole fraction of component i in vapour stream leaving n'th stage

$Z_{n,i}$ - mole fraction of component i in VPCE/LPCE gaseous stream leaving n'th stage

Subscripts

i - component index

n - stage index

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