HEAVY WATER UPGRADER DYNAMIC SIMULATION (UGDYNSIM)

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1.0 INTRODUCTION

Water distillation columns, operating under vacuum, are widely used to separate light water from heavy water. In CANDU nuclear stations, they are used to upgrade low purity heavy water (recovered via the liquid collection and vapour recovery systems) to reactor grade and are referred to as *Heavy Water Upgraders*. Reactor grade heavy water is recycled to the appropriate reactor systems and the D_2O depleted light water is rejected via the active liquid waste discharge system. Since the isotopic concentration of the recovered heavy water changes frequently, the concentration of D_2O in the feed to the upgraders is not constant and the upgraders are never operated under steady state conditions. The existing upgrader process simulation model, UGSIM[1], is a steady state model that uses binary approximation to simulate H/D separation. The UGSIM code, therefore, is only capable of giving *the end point of the operating trajectory from the previous feed composition to the new feed composition*. Thus, for an upgrader under normal operation, this provides only a rough approximation of the reality.

Ontario Hydro has now developed an upgrader dynamic simulation code (UGDYNSIM), with a point and click Microsoft WINDOWS 95 or WINDOWS NT user interface, that will predict the time dependent performance of the upgraders. The UGDYNSIM is a rigorous distillation model that accounts for the oxide forms of H, D and T (i.e., all the six water species). A fast 32-bit program has been used to simulate systems of any size, with multiple interlinked columns. The user specifies the number of theoretical stages, column pressure profile, reboiler duty, system inventory, feed composition etc. The simulation can be continuous or in specified time-steps.

The UGDYNSIM program is the most sophisticated heavy water distillation simulation program in existence today. This paper presents the features and capabilities of UGDYNSIM.

2.0 SPECIAL FEATURES OF WATER DISTILLATION

As compared to the simulation of distillation columns in the petrochemical industry, water distillation column simulation presents special difficulties.

- Water distillation is an isotope separation process characterized by very slight differences in relative volatility between the species being separated.
- The degree of separation in a typical water distillation column used for heavy water upgrading or production is very high.

- The relative abundance of H_2O to D_2O as measured by the H:D ratio can change by six or more orders of magnitude from the top of the column to the bottom of the column.
- The number of theoretical plates in a water distillation column is usually 400 or more. By comparison, a large distillation column in the petrochemical industry has 40-50 plates.
- Water distillation involves the additional complication of the following rapid equilibration reactions in the liquid phase:

$$H_2O + D_2O \Leftrightarrow 2HDO$$
$$H_2O + T_2O \Leftrightarrow 2HTO$$
$$D_2O + T_2O \Leftrightarrow 2DTO$$

The equilibrium constant for these reactions is approximately 4, which is the ideal value based on a statistical rearrangement of the H, D and T atoms. Since in most applications, the T_2O concentration is extremely low, tritium (T) is primarily found in the HTO and DTO species. Because of the equilibration reactions, water distillation is reactive distillation.

Due to these special features, water distillation cannot be properly simulated by a simulation code developed for the petrochemical industry. There are only a few proprietary water distillation codes in existence, with the most rigorous and sophisticated ones developed by Ontario Hydro.

3.0 DISTILLATION COLUMN THEORY

The component mass balance equations for a water distillation column with fixed inventory (mole) per theoretical stage are expressed by the well known tridiagonal matrix equations:

$$\frac{dq_{i,n}}{dt} = f_{i,n} - a_{i,n}x_{i,n-1} - b_{i,n}x_{i,n} - c_{i,n}x_{i,n+1}$$

for $i = 1 \ldots, m$ and $n = 1 \ldots, N$, where m is the number of components, N is the number of theoretical plates or stages, $q_{i,n}$ is the stage inventory (mole) of component i for stage n, $x_{i,n}$ is mole fraction, $f_{i,n}$ is feed rate (mole/s), and the coefficients $a_{i,n}, b_{i,n}, c_{i,n}$ are defined as:

$$a_{i,n} = L_{n-1}$$
$$b_{i,n} = -L_n - D_n^L - K_{i,n}(V_n + D_n^V)$$
$$c_{i,n} = K_{i,n+1}V_{n+1}$$

where

L_n = liquid flow leaving stage n (mole/s),
V_n = vapor flow leaving stage n (mole/s),
D_n^V = vapor product flow leaving stage n (mole/s),
D_n^L = liquid product flow leaving stage n (mole/s),
$K_{i,n}$ = vapor-liquid equilibrium ratio for component i on stage n (dimensionless),

The differential equations described above must be integrated numerically. For absolute stability, an implicit Euler method is used in UGDYNSIM. The accuracy of the numerical integration improves for small time steps. However, smaller time steps require more computation time to simulate a given simulation scenario. The step size can be experimented with to determine the appropriate size. If reducing the step size by a factor of two makes an insignificant difference to the simulation results, then the step-size is small enough for practical purposes.

4.0 LIQUID-VAPOR EQUILIBRIUM RELATIONS

For water distillation, the vapor liquid equilibrium ratio calculation assumes an ideal solution of water species. Therefore,

$$K_{n,i} = \frac{p^*_{i,n}}{P_n},$$

where $p^*_{i,n}$ is the vapor pressure of pure component i at the temperature of stage n and P_n is the absolute pressure of the stage.

For water distillation, the assumption of ideal solutions is generally accepted as being very accurate. The vapor pressure calculations in UGDYNSIM are based on the procedure described in the paper by W. Alexander Van Hook. [2]

5.0 BENEFITS OF DYNAMIC PROCESS SIMULATION

Dynamic simulation of a complex process system is valuable because it provides insight into system operation that is difficult to obtain even with field experience. For example, in unsteady state operation of a heavy water upgrader, the head product and bottom product variations with time are a complex function of feed composition, control actions, and many other process variables, including past history. The complexity is such that hand calculations are of limited value, and "intuition" based on experience is only a very crude guide as to what operating performance can be expected. The benefits of the dynamic process simulation code are as follows:

- Realistic process model (Current UGSIM Steady State Model is only a very rough approximation of reality);

- Allows simulation of automatic control to evaluate its potential benefits and assess control strategies;

- Accurately predicts time required to achieve desired column profile under total reflux and normal operation modes;

- Allows evaluation of different operating scenarios and optimization of operational strategy;

- Increased plant efficiency due to a better understanding of the process system operation;

- Provides improved troubleshooting and diagnostic capability;
- Useful as a training tool (The user friendly program interface promotes faster learning by new users, greater use by existing users, and continuity through staff turnover);
- Integration of program with on-line process control system;
- Permits performance monitoring of upgrader packing under dynamic operating conditions.

Within the heavy water upgrader distillation columns, saturated vapor flows up and is contacted with liquid which flows down the column by gravity. The columns are packed with copper/bronze packing material which provides a large surface area for contacting downward flowing liquid with upward flowing vapor. The separative power of a column is characterized by its number of theoretical plates (NTP). The terms "theoretical stages", theoretical trays" and "theoretical plates" are often used interchangeably. The packing efficiency is characterized by the Height Equivalent to a Theoretical Plate (HETP), which is the height of packing required to provide the amount of separation equivalent to a theoretical plate. Usually under steady state operating conditions (i.e., the column pressure, reboiler boil-up rate, feed concentration, feed rate and product draw-off rates are maintained constant for at least two or three days), the top and bottom products concentrations are determined by sampling and analysis. With the use of steady state simulation codes (such as UGSIM), the actual number of theoretical plates (NTP) are determined. From the total packing height in the columns and the estimated NTPs, the HETP is calculated. Due to the large water inventory in the columns (several megagrams), it normally takes about 7 to 10 days of operation to achieve near steady state. Stations seldom have the large inventory of the required feed stock of the same feed concentration to carry-out such a lengthy packing performance assessment. Periodic packing performance monitoring is becoming increasingly important, since the corrosion of the packing material (due to impurities in the feed water) has the effect of slowly deteriorating the packing efficiency. With the use of the dynamic simulation code, the performance monitoring can be carried-out under total reflux or normal operation, without the lengthy wait to achieve steady-state. The only requirements are constant pressure and boil-up rate.

6.0 FEATURES AND CAPABILITIES OF THE UGDYNSIM

6.1 Development of UGDYNSIM Code

The UGDYNSIM dynamic simulation code is designed to run on PC computers under the 32-bit Windows 95, Windows NT or compatible operating systems. The program allows the user to setup and run upgrader operation simulation scenarios in a flexible manner with a point and click Windows 95 or Windows NT user interface.

The UGDYNSIM simulation program is descended from the FLOSHEET code [3], UGSIM code [1], DYNSIM code [4], and Single Column Generic UGDYNSIM [5] code. The FLOSHEET and UGSIM codes are steady state codes developed by Ontario Hydro starting in 1984, and both these codes are still widely used today. The fully dynamic DYNSIM and Single Column Generic UGDYNSIM were developed for Ontario Hydro by NITEK Corporation after 1990. The dynamic distillation column algorithms in UGDYNSIM are very similar to those in CFSTIM [6] developed by the Canadian Fusion Fuels Technology Project (CFFTP), a dynamic simulation code used internationally for the International Thermonuclear Experimental Reactor (ITER) project.

6.2 UGDYNSIM Program Features

UGDYNSIM is a realistic upgrader process model that accurately determines the time required to achieve desired column profile under total reflux and normal operation modes. It allows study of control strategies and simulation of automatic control to evaluate its potential benefits. Different operating scenarios can be evaluated to optimize the operational strategy. It is an extremely useful tool for upgrader operator training. It provides flexibility for future integration of simulation program with on-line process control system.

6.2.1 Main Window. When the program is started, the Upgrader page is displayed in the main window. A typical main window for a moderator upgrader is shown in Figure 1. The main window is configured to mimic the station upgrader system, including all the major equipment and feed valve locations.

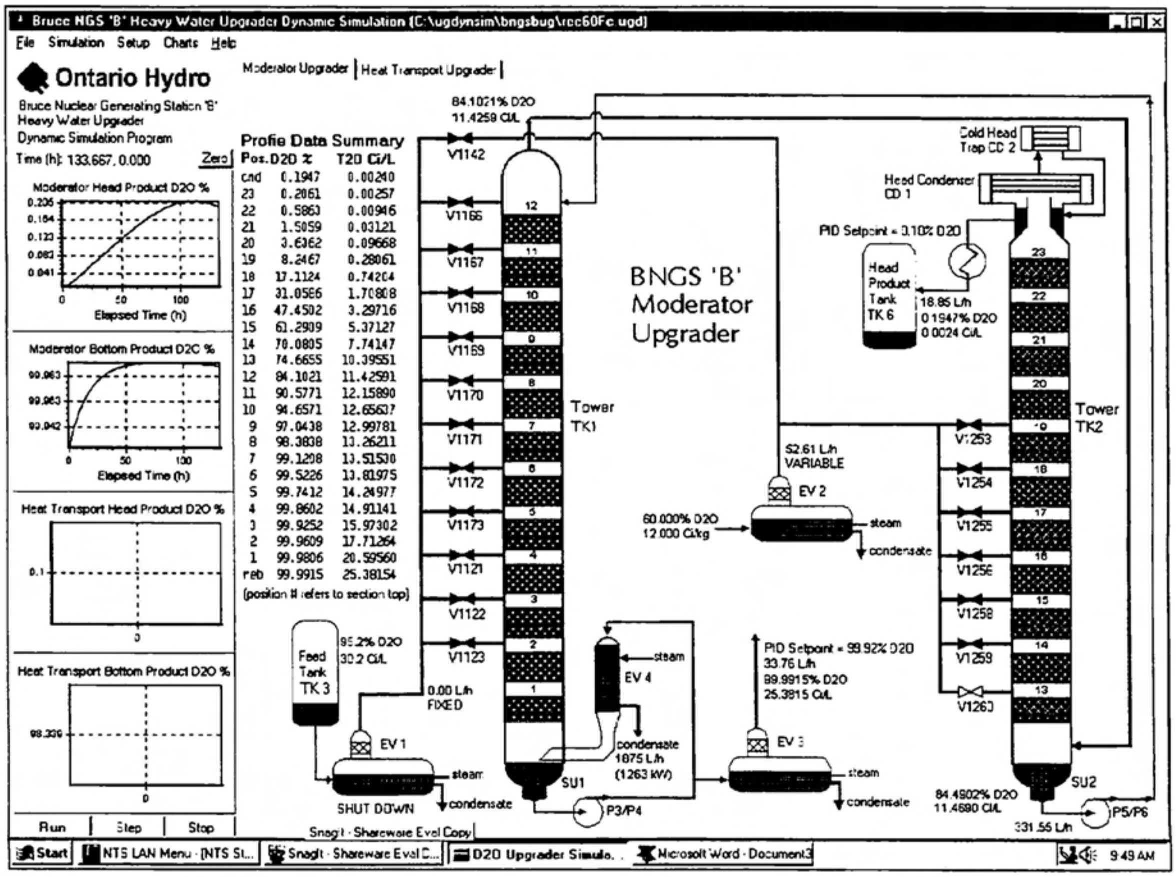

Figure 1: UGDYNSIM Main Window Showing Bruce NGS 'B' Moderator Upgrader Mimic Panel.

The simulation may be setup, started, stopped and restarted at any time, with control system adjustments made via mimic screen, just like with a real control console. Extensive error checking and meaningful error messages keep the user on track. The user is notified about missing or erroneous data and prompted for the correct inputs.

Four charts are preconfigured along the left side of the screen:

- moderator upgrader head product D_2O %
- moderator upgrader bottom product D_2O %
- heat transport upgrader head product D_2O %
- head transport upgrader bottom product D_2O %

At the bottom left hand corner of the screen are three buttons Run, Step and Stop, which are used for starting, stepping and stopping a simulation run. Clicking on Run starts a simulation to run continuously until the Stop button is pressed. Clicking on Step causes the simulation to proceed only one integration time step.

The Zero button just above the four charts zeroes the time simulation time.

The File, Simulation, Setup, Charts and Help menus are used to load/save simulation cases, control the simulation run, setup the simulation, view charts, and get program help. These menus are described in more detail later.

Clicking on the Heat Transport Upgrader page tab changes the page to the Heat Transport Upgrader mimic panel, which is similar to the Moderator Upgrader mimic panel. A typical main window for a heat transport upgrader is shown in Figure 2.

Generally, clicking on an equipment tag will bring up a dialog to configure the equipment. For example, clicking on the feed evaporator EV-2 tag on the moderator upgrader mimic will bring up a dialog, so that input data can be entered or edited (Figure 3). Clicking on the V1172 tag on the moderator upgrader mimic will bring up a valve open/close dialog to confirm the status of the valve. Closed valves are colored amber, while open valves are colored white. Generally, two connected feed valves cannot be open simultaneously. When valves are opened and closed, simple consistency check logic ensures physically reasonable operation.

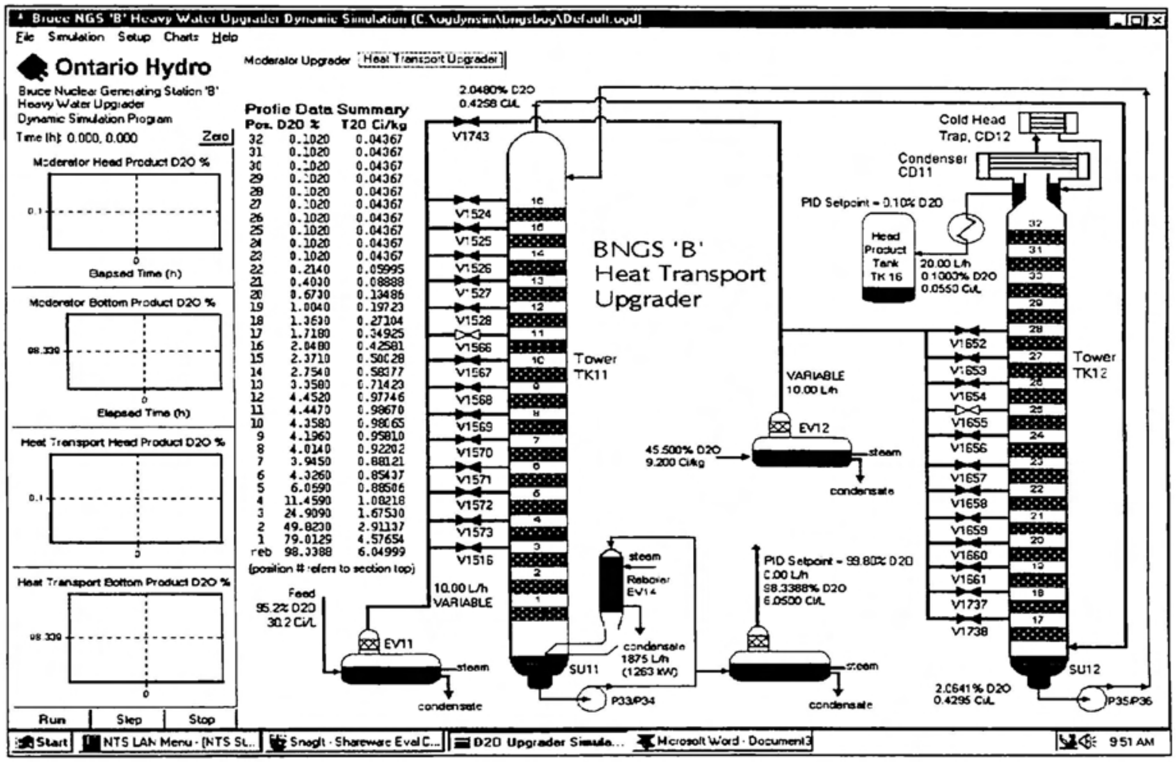

Figure 2: UGDYNSIM Main Window Showing Bruce NGS 'B' Heat Transport Upgrader Mimic Panel.

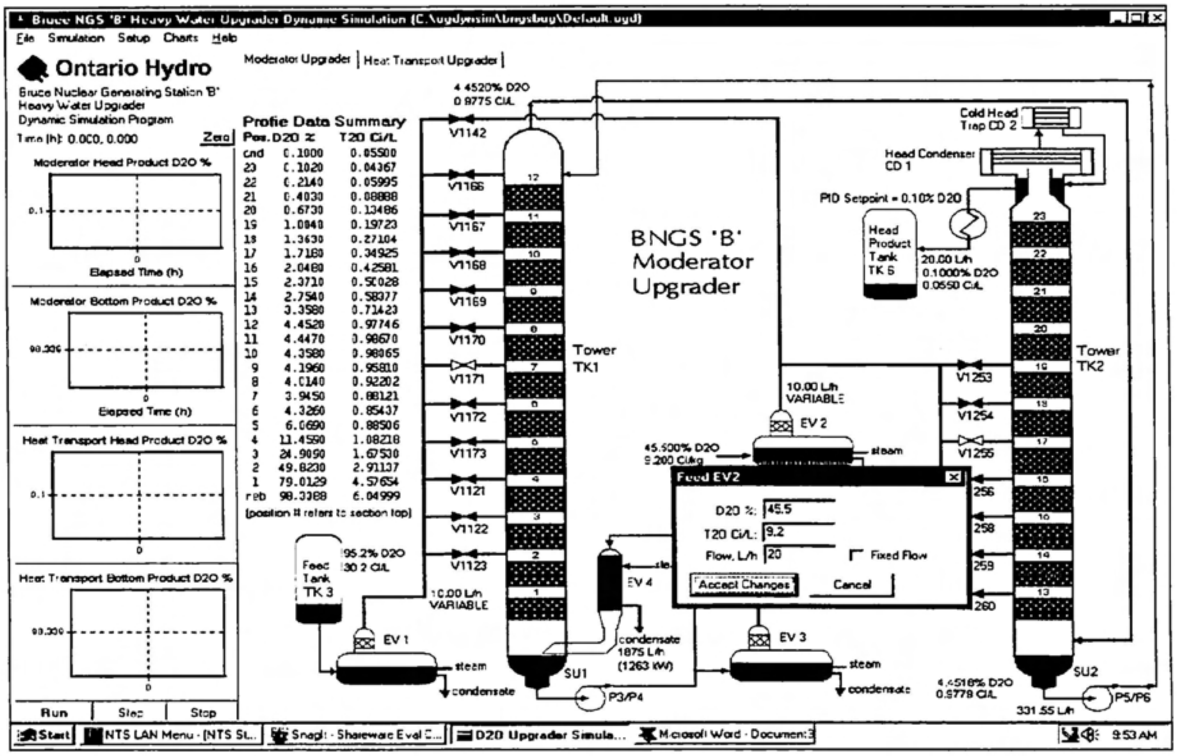

Figure 3: UGDYNSIM EV2 Dialog Shown When Clicking EV2 Tag

6.2.2 SetUp Menu. Selecting the SETUP menu (shown in the top left-hand side of Figure 1) brings up the upgrader setup dialog shown in Figure 4. The setup dialog allows user input of upgrader configuration data. The user specifies the reboiler and condenser data such as pressure, temperature, flowrates and inventory. For each packed section of the upgrader, the user specifies the number of stages, top and bottom pressures, top and bottom D_2O and T_2O concentrations, water inventory in the packing, and water inventory in the tower sumps and the distributors (sump inventory). The top and bottom pressures, and D_2O and T_2O concentrations for each section can be set based on station operating data and sampling and analysis. If such information is not available, these values can be based on linear extrapolation of the overall tower top and bottom values. This capability to specify the parameters of each section is a very useful feature of UGDYNSIM, since this allows the user to simulate the effect of loss of efficiency in some sections on the upgrader performance. For example, if the liquid distributors in some sections are partially or completely plugged, the liquid maldistribution will result in loss of separation efficiency. Several simulations can be run using different number of stages in these sections. By comparing the simulation results with the actual operating data, the number of stages in the plugged sections can be predicted. Using the predicted number of stages, simulations can then be carried-out to optimize the operation strategy, until future maintenance shutdown.

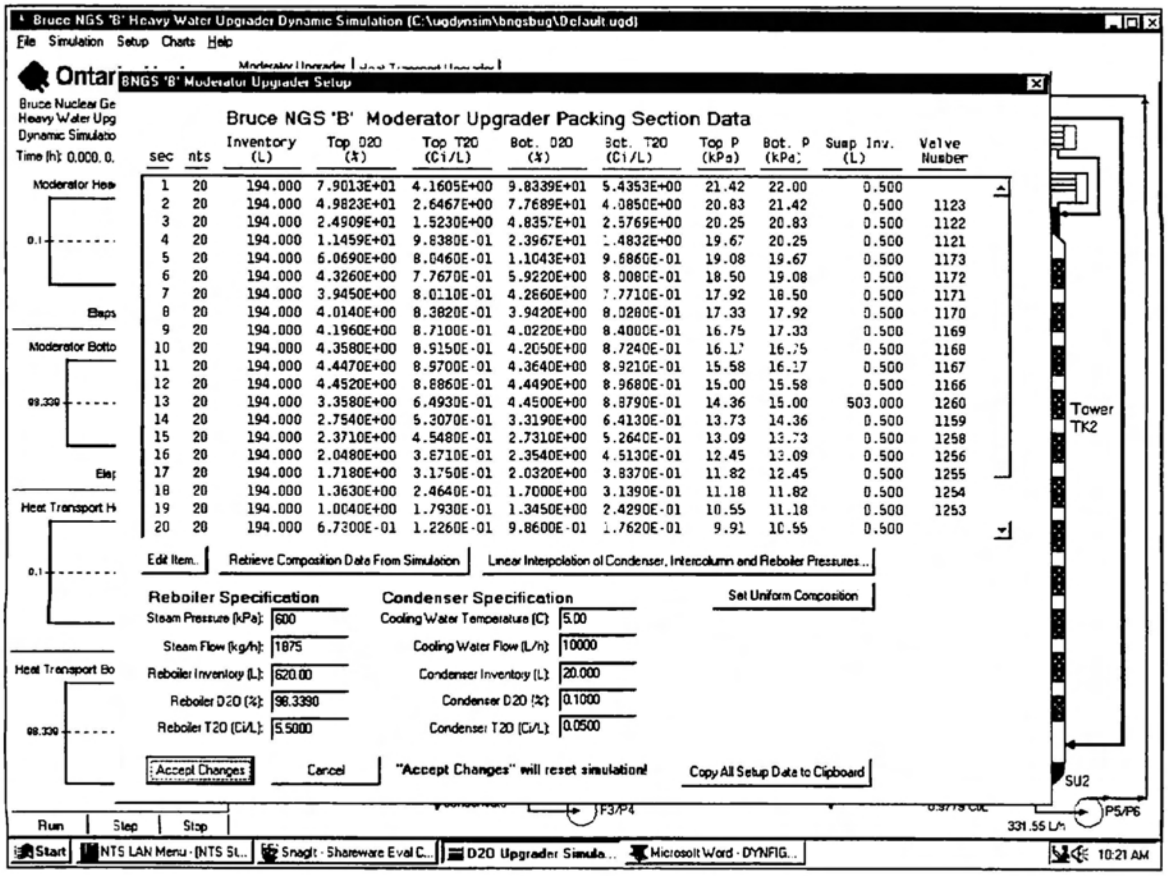

Figure 4: Moderator Upgrader Setup Dialog.

6.2.3 Control Algorithms Menu. Selecting the Control Algorithms menu brings up the Control Algorithm Setup dialog, as shown in Figure 5. For each of the product streams, the user may set the control mode to Fixed Flow, Fractional Flow, or PID Control. This feature permits simulation of automatic control to evaluate its potential benefits and assess control strategies.

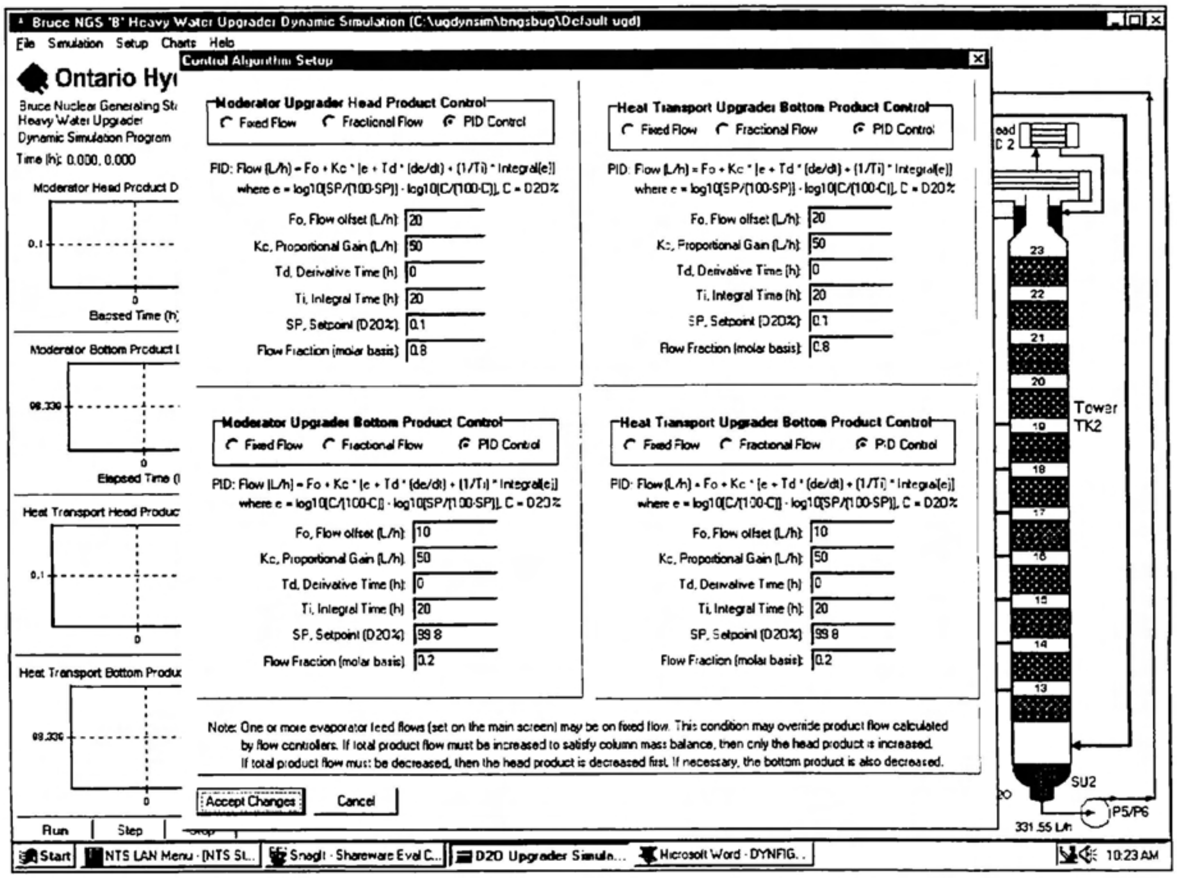

Figure 5: Control Algorithm Setup Dialog.

6.2.4 Charts Menu. The Charts Menu brings up preconfigured charts for the following parameters:

- D_2O and T_2O concentration profiles
- Column temperature and pressure profiles
- Trends of column head and bottom product D_2O and T_2O concentrations with time
- Trends of feed and product flow variations with time
- Trends of inter-column sump D_2O and T_2O concentrations with time.

The charts can be refreshed (animated) automatically while the simulation is running, so that the user can see the change in the profiles with time. The Charts Menu is context sensitive, in that the moderator upgrader charts are invoked if the moderator mimic page is on top, or the heat transport upgrader charts are invoked if the heat transport upgrader mimic page is on top.

7.0 SIMULATION OF THE START-UP OF THE BRUCE 'B' MODERATOR UPGRADER

In this example, the Bruce 'B' Moderator Upgrader, consisting of two towers, is assumed to be operated using 5.59 Mg of 60% D_2O inventory with a tritium concentration of 12 Ci/kg-feed. The Upgrader is started in the total reflux operating mode from the shutdown state. The Upgrader is assumed to have a uniform isotopic profile in both towers at start. The isotopic target for the Head Product (HP) is 0.1% D_2O. Normal feed will be resumed, when this target is reached, with only HP drawoff. Bottom Product (BP) drawoff will resume only when reactor grade D_2O isotopic is achieved. The BP isotopic target in this example is 99.92% D_2O. The assumed total number of stages in the two towers is 460.

In the total reflux operating mode, the HP isotopic will start to decrease and the BP isotopic will increase. Figure 6 shows that the HP isotopic reaches its target setpoint (0.1% D_2O) after 42 hours of Upgrader operation in total reflux. Therefore, removal of HP from the upgrader can start at this time, if feed is also introduced. However, after 42 hours, the BP isotopic is still about 93% D_2O. Hence the BP draw-off cannot yet be started.

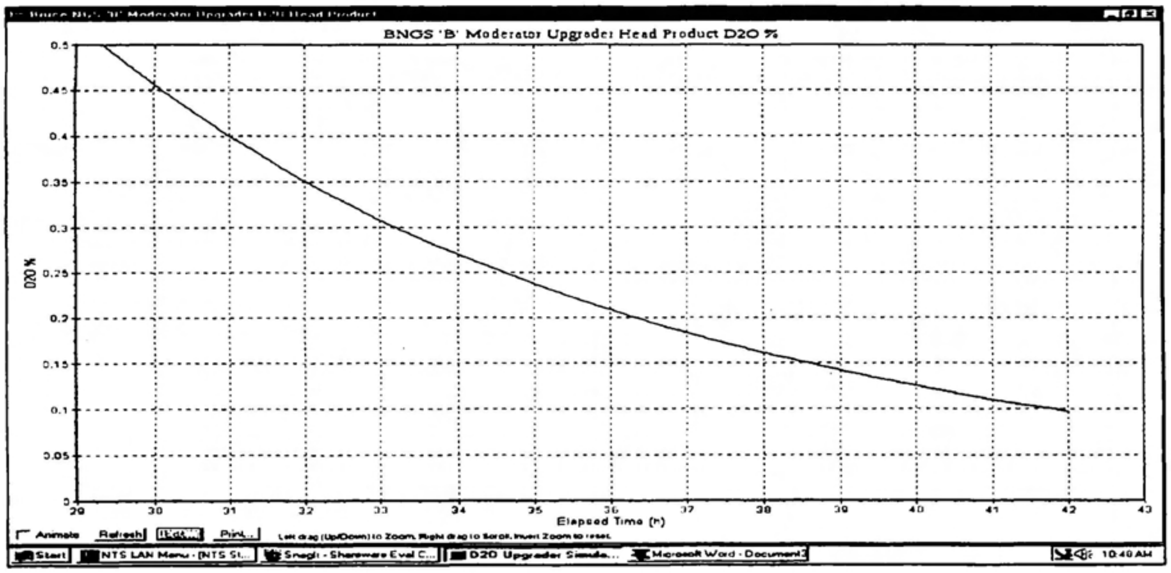

Figure 6: Variation of Head Product Isotopic With Time

When feed is introduced, establishing the HP flow will remove H_2O from the Upgrader. This allows the isotopic profile in the upgrader to build such that reactor grade D_2O can later be removed as Upgrader BP. Through the simulation, it is found that the feedrate to the Upgrader should be initially set at about 29 kg/h. To maintain the upgrader mass balance, the HP is drawn at a rate equal to the feed rate. Operation in this mode will continue until the BP reaches its isotopic target specification of 99.92% D_2O. As shown in Figure 7, this occurs 77 hours after the HP flow was started or 119 h (77 hours + 42 hours) after the initial Upgrader startup in total reflux. The BP draw-off can now be started.

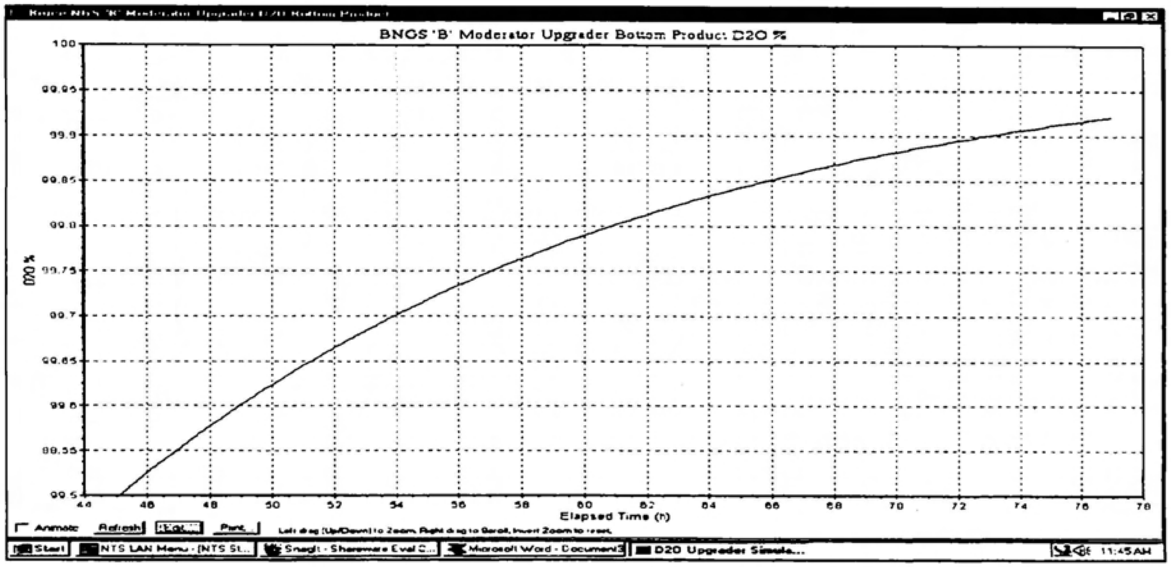

Figure 7: Variation of Bottom Product Isotopic With Time

With both the HP and BP isotopics having reached their respective setpoints, flow control of Upgrader HP and BP is assumed to be placed on automatic PID control. Isotopic setpoints to the PID controllers are as noted above. The isotopic trends for the HP and BP are shown in Figures 8 and 9 respectively. It is evident from these figures that further fine tuning of the PID controller parameters is required to stabilize the product isotopics. Further optimization of the control parameters to improve the stability of the Upgrader product isotopics will be performed in the near future.

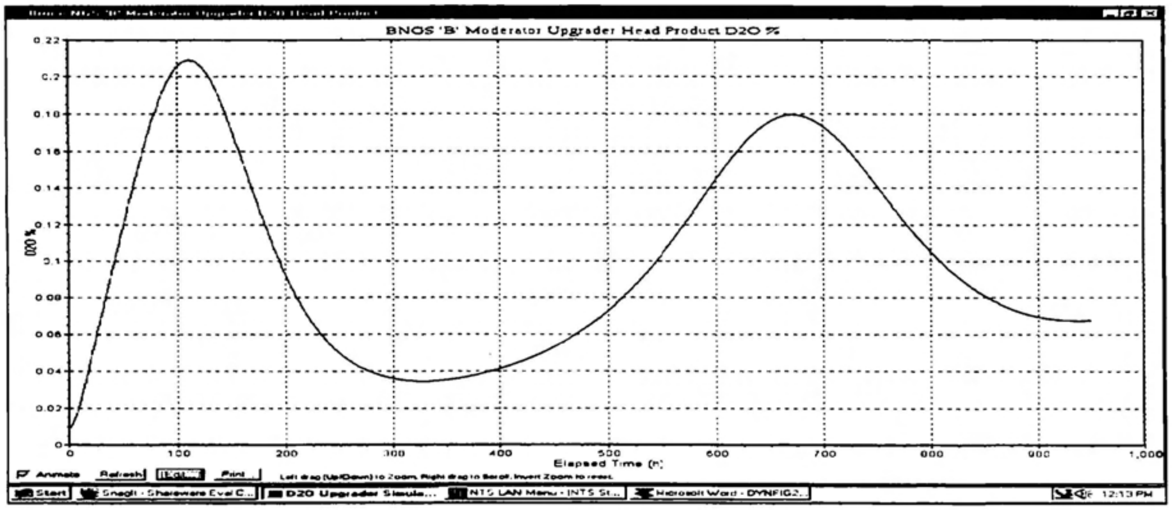

Figure 8: Trend of Head Product Isotopic Using PID Controller

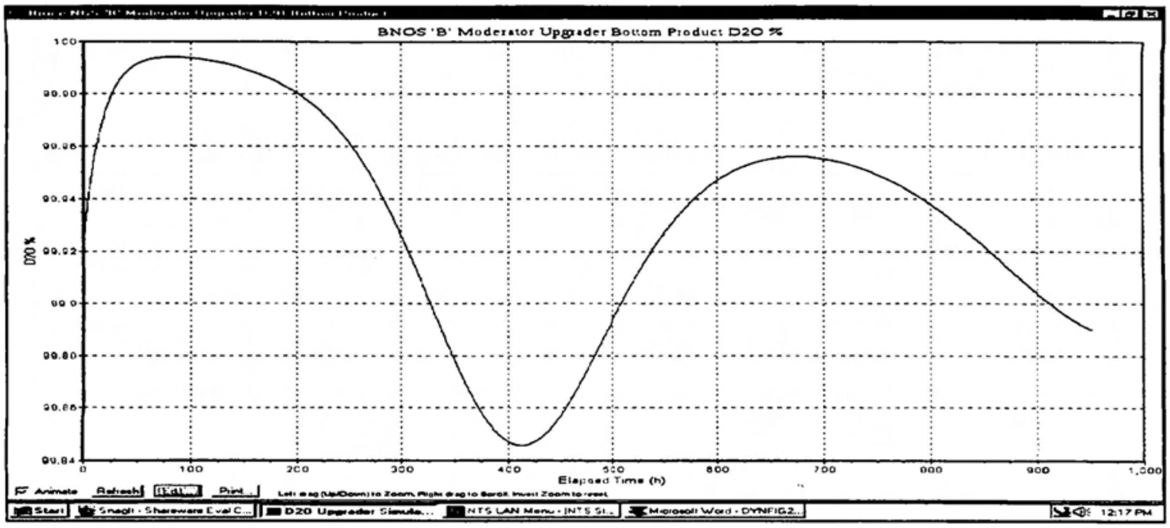

Figure 9: Trend of Bottom Product Isotopic Using PID Controller

The Upgrader Feed, HP and BP flowrates are shown in Figure 10.

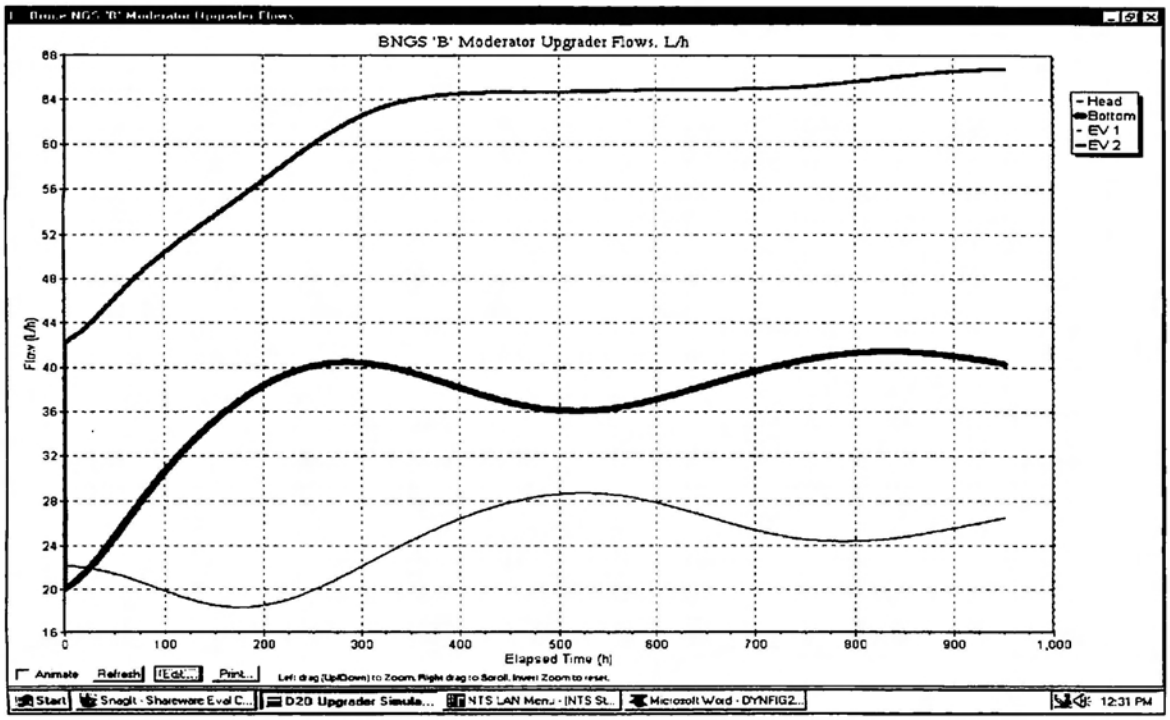

Figure 10: Trends of Head Product, Bottom Product and Feed Flowrates

Additional information obtained from this simulation are:

- The final upgrader feedrate is about 66 kg/h.
- Upgrader tower D_2O isotopic profiles to determine the correct feed valve location. For the above example, the optimum feed valve is V1260 (located above the packing section # 13).

The user can also extract other output data from UGDYNSIM as discussed in Section 6.0.

8.0 FUTURE PLANS

Customized versions of UGDYNSIM have been developed for some of the Ontario Hydro heavy water upgraders (at Bruce NGS B and Pickering NGS). It is anticipated that by 1998 all Ontario Hydro heavy water upgraders will have customized versions of UGDYNSIM. Extensive testing and calibration of the code using station operating data will be carried out in the near future.

9.0 REFERENCES

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