Photocopy Request for: Victoria Romero

Copied by: Cheyenne **Date copied:** 08/20/2003

S C I E N C E S T A R T S H E R E

RESEARCH LIBRARY

photo@lanl.gov -- 505-667-4175

Document Delivery Service

Please use the Journal Article request form at: http://lib-www.lanl.gov/requests.htm
Or via LinkSeeker in our LANL databases

In-House Document Delivery Service. Copies are provided from materials in the Library's collection (journals, books, conference papers, etc). (**Exception**: We do not make copies of/from standards and codes.) Copying is done in compliance with the copyright law (see notice above) and with Library policy (see following).

Policies – The Research Library:

- Will copy journal articles, excerpts from books, or conference papers constituting 20% or less of the journal issue, book, proceedings volume (by page count).
- Will not facilitate systematic copying from a journal issue, book, or proceedings volume (i.e., requesting one article one day and another the next day, week, etc.).
- Will not provide multiple copies of any journal article, book excerpt, or conference paper.

For requests we cannot honor:

- Please consult with a librarian concerning possible alternatives.

Obtaining Photocopies from External Sources. The library uses a vendor to obtain photocopies from materials not owned.

If collection materials are unavailable due to binding, missing, etc.:
Non-rush: order at library's cost
Rush: order at your cost

Note: This is a highly requested service. Turn around times varies from 2 to 5 days (please include delivery/mail time). Extensive lists may require additional time.

Date: Mon, 11 Aug 2003 09:30:06 -0600
To: photo@lanl.gov
From: ROMERO ANGELICA VICTORIA <avr@lanl.gov>
Subject: 174435-1060615806
X-Mailer: Research Library request.cgi 1.2
X-Scanned-By: MIMEDefang 2.35

EIS Name: ROMERO ANGELICA VICTORIA
EIS Znumber: 174435
EIS Group: C-SIC
EIS MS: J514
EIS Phone: 505-667-7520
EIS Fax: 505-667-9905
EIS Email: avr@lanl.gov

Citation: Paffett, M.T.,
Surface Characterization of TFTR First Wall Graphite Tiles Used During DT Operations,
Fusion Science and Technology,
41(3), 1131-1136

Month needed: Aug
Day needed: 18
Year needed: 2003
Delivery method: Email
Language: English only
Journal availability: Send the article only if it is in the Library collection
Read copyright agreement: Yes
Form: Submit Journal Article Request

STEADY-STATE COMPUTER MODELING OF A RECENT H-D-T CRYOGENIC DISTILLATION EXPERIMENT AT TSTA

Jennifer S. Young, Robert H. Sherman, R. Scott Willms*
Los Alamos National Laboratory
P. O. Box 1663
Los Alamos, NM 87545, USA
1-505-667-5802

Yasunori Iwai and Masataka Nishi
Japan Atomic Energy Research Institute
Tritium Engineering Laboratory
Tokai-mura, Naka-gun, Ibaraki-ken, 319-1195, Japan
81-29-282-6390

ABSTRACT

Cryogenic distillation is the only technique with the capacity to handle the hydrogen isotope separation requirements of a fusion power plant. However, there are safety and cost considerations associated with the considerable tritium inventory that can accumulate in such an isotope separation system (ISS). The ISS must be able to reliably produce specified products while responding to varying input streams. To design an ISS that balances all of these considerations and operate it reliably, it is essential to have a computer model of the system. This allows for a better understanding of the system and the exploration of various parameter regions that would otherwise require very expensive experimentation.

The value of such a model, however, is questionable until it is validated by comparison with actual experiments. Recently, as part of the Annex IV US/Japan collaboration, a series of tests were conducted on the ISS system at the Tritium Systems Test Assembly (TSTA) located at Los Alamos National Laboratory (LANL). This system has a fusion power plant-relevant capacity of 6 SLPM (standard liters per minute). These experiments employed light hydrogen (protium), deuterium and tritium. Conditions at five steady state conditions were measured. The measurements included concentration measurements at the column feed, top and bottom, and also at intermediate points.

These measurements served as a benchmark for comparison to DYNSIM, the model that has been in use at LANL for many years.† This model was able to accurately predict the column concentration profile based on the measured pressure, temperature, reboiler heat, feed composition and flows for a set of significantly different operating conditions. These results impart confidence that the model is useful for future ISS design and for better understanding of existing system operations.

I. INTRODUCTION

Cryogenic distillation is the only technique with the capacity to handle the hydrogen isotope separation requirements of a fusion power plant. However, there are safety and cost considerations associated with the considerable tritium inventory that can accumulate in such an isotope separation system (ISS). The ISS must be able to reliably produce specified products while responding to varying input streams. To design an ISS that balances all of these considerations and operate it reliably, it is essential to have a computer model of the system. This allows for a better understanding of the system and the exploration of various parameter regions that would otherwise require very expensive experimentation.

The value of such a model, however, is questionable until it is validated by comparison with actual experiments. Recently, as part of the Annex IV US/Japan collaboration, a series of tests were conducted on the ISS system at the Tritium Systems Test Assembly (TSTA) located at Los Alamos National Laboratory (LANL). This system has a fusion power plant-relevant capacity of 6 SLPM (standard liters per minute). These experiments employed light hydrogen (protium), deuterium and tritium. Conditions at five steady state conditions were measured. The measurements included concentration measurements at the column feed, top and bottom, and also at intermediate points.

A number of ISS computer models have been developed[1-2]. For the present study, these measurements performed served as a benchmark for DYNSIM, the model that has been in use at LANL for many years.† This model was able to accurately predict the column concentration profile based on the measured pressure, temperature, reboiler heat, feed composition and flows for a set of significantly different operating conditions. These results impart confidence that the model is useful for future ISS

* Address correspondence to this author

† This code, originally at Mound Laboratory and referred to as DTL, was transferred by Bill Rutherford to Robert Sherman at LANL in the late 1970's. As the code further developed at LANL, it was renamed to DYNSIM, and it has been referenced by that name in interactions LANL has had with a number of laboratories. However, the LANL code should not be confused with a code bearing the same name which has been used at Ontario Hydro.[1]

design and for better understanding of existing system operations.

II. EXPERIMENTAL

For this study, only ISS column I, the first column in the TSTA four-column cascade was cooled. This system, depicted in figure 1, has been described previously.[3-7] The experimental campaign which is the subject of this paper was started by loading ISS column I with 19.9 moles of diatomic hydrogen isotopes consisting overall of 37.4% H, 55.5% D and 7.1 % T. Column I operating conditions were set. The parameters of primary importance were reboiler duty; feed, bottoms and distillate flowrates; feed stage number; reboiler liquid level and pressure. Column product streams were remixed, isotopically equilibrated and fed back into column I. The amount of inventory outside of column I was kept to a minimum. After a matter of hours, a steady-state condition was achieved as observed by unchanging product compositions. At that point column compositions were measured using on-line Raman spectroscopy at the feed stream, the two products streams and at side-stream positions along the column (stage numbers given later).

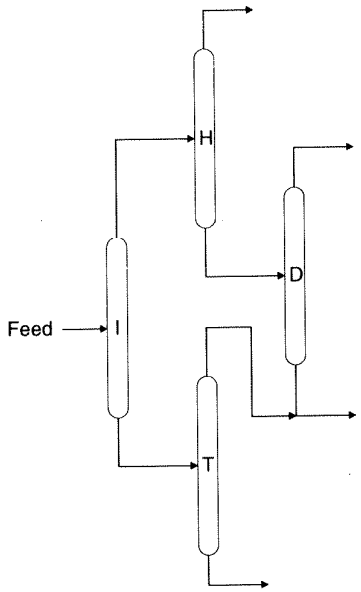

Figure 1 TSTA ISS four-column cascade

Once a case was complete, a new set of conditions were set, another steady-state was achieved and another set of concentration measurements was collected. In this manner a total of five case datasets were collected. Between cases 3 and 4, the amount of gas in the ISS was changed by offloading a measured amount of gas from the top of column I. Thereafter, remaining in the column were 14.8 moles of diatomic hydrogen isotopes consisting of 29.4% H, 61.0 % D and 9.6% T.

The process settings for each of the five cases are summarized in Table 1.

III. MODEL DESCRIPTION

The DYNSIM program was written to model the performance of a hydrogen isotope cryogenic distillation system. A single column, or a series of interlinked columns can be modeled. The model is useful for ISS designs and for interpreting results from experiments. Both steady state and dynamic operations can be modeled. Multiple columns may be interconnected freely and return streams are permitted. Isotopic equilibration may be provided where necessary for an entire feed stream or on individual stream components, if multiple streams are mixed. Internal reboilers, one per column, may be simulated for optimization of large diameter, high throughput columns. In general it is assumed that continuous flow is desired with matched feed and product streams. Optionally the code can simulate a single batch distillation column with a fixed initial charge. The code, for instance, has been used previously to model the dynamic performance of a column which incorporates the recycle of an equilibrated side-stream to improve performance.[8]

The code has the capability of considering the hydrogen isotope vapor-liquid equilibrium to be either ideal, or to take into account partial or full non-ideality. Real molar volumes and heats of vaporization are utilized.

The data that are input to the simulation are the feed composition, the distillate flowrate, the bottoms flowrate, column temperature and pressure, and reflux rate or reflux to distillate ratio. In the cases presented here, the reflux rate was not measured directly; therefore, the reflux rate was set to obtain a reboiler duty that matched the value measured during the test runs. As stated earlier, during the experiment the distillate and bottoms were recycled to the feed and equilibrated before reentering the column.

IV. RESULTS AND DISCUSSION

Input into DYNSIM were the column I specifications, namely a single column, 2.84 cm in diameter, 83 theoretical stages (Stage 0 is the reboiler and stage 83 is the condenser) and an HETP (height equivalent of a theoretical plate) of 5.08 cm. The feed compositions and process conditions listed in Table 1 were input into the code for each case.

Case 1 is the first steady-state condition. The model results (lines) and the measured experimental compositions

(markers) are shown on figure 2, where the mole fraction is plotted against the stage number for each of the six hydrogen isotope species. The agreement between model and experiment is excellent.

For case 2, the distillate rate was doubled while the bottoms rate was halved and the reboiler duty remained constant. This resulted in operation with half the reflux ratio of case 1 which should result in poorer separation. Indeed, the concentration profiles for case 2, shown on figure 3, are less sharp compared to case 1. Also, increasing the amount of material leaving the top while reducing the amount leaving the bottom should move the composition profiles up the column. This is also observed, especially in the position of the maximum HT composition. Good agreement is observed between model and experimental concentrations at all points for case 2.

For case 3, the distillate rate and bottoms rate are both lowered to 40% of the case 1 values while the reboiler duty remained approximately constant. This results in a reflux ratio approximately 2.5 times higher than case 1. This should result in sharper concentration profiles within the column, and indeed this is observed for the case 3 results as shown on figure 4. The ratio of distillate product to bottoms product is same between cases 1 and 3 so the position of material within the column should be similar. Indeed this is the case with this especially apparent by comparing the position of the HT concentration maximum. Excellent agreement is observed between model and experimental concentrations of all case 3 points.

For case 4, a major change was made to the column to quickly move to very different parameter space. The amount of material in the column was reduced, and, since material was removed only from the top, the relative amount of each isotope species was changed. With less material in the column, the reboiler liquid level would have dropped to zero. Thus, the reboiler duty was decreased to about 50% of its previous setting. This resulted in a reasonable liquid level by reducing the amount of liquid held-up on the column packing. Also, the feed stage was moved up the column to stage 47. Flowrates were not changed compared to case 3. At the new operating condition the reflux ratio was cut approximately in half (going from case 3 to case 4). This should make the concentration profiles in the column less sharp. Indeed this is apparent by inspecting the results for case 4 shown on figure 5. Also, it is observed that the profiles are moved up the column as they should since the feed was moved higher. Even with these major changes, there is still good agreement between the experimental and model results for case 4.

For the final test, case 5, the only change was a doubling of the distillate rate. This cut the reflux ratio in half (compared to case 4). This should make the concentration profiles less sharp. Indeed this is observed by inspecting the results for case 5 on figure 6. It is observed that the HT profile is now slurred across the entire height of the column. Doubling the amount of material removed from the top of the column while holding the bottom product rate constant should also move the concentration profiles higher in the column. Comparing cases 4 and 5, this is observed most clearly for the HD concentration. There is excellent agreement between the experimental and model results.

The experimental concentration values that are shown on figures 2-6 are also present in tabular form in Table 2.

V. CONCLUSIONS

The TSTA ISS column I was operated at five significantly different, fusion power plant relevant conditions. It was observed that the column responded as it should. Concentration profiles became sharper as reflux ratio was increased. The profiles moved higher in the column as the ratio of material removed from the top was increased relative to the bottom, and as the feed stage was moved higher in the column.

DYNSIM was used to model these experiments. There was excellent agreement between the model and experimental results. The only exception to this was one set on concentration measurements in case 1, and this mismatch was probably due to a leaking valve which inadvertently mixed material from two locations.

Based on these results it is concluded that the LANL DYNSIM code can accurately model the steady state behavior of a hydrogen isotope cryogenic distillation system.

REFERENCES

1. A. Busigin and S. Sood, "Steady-State and Dynamic Simulation of the ITER Hydrogen Isotope-Separation System," *Fusion Technol.* **28(3)**, 544-549 (1995).
2. M. Kinoshita, "Simple-Model for Dynamic Simulation of Stage Separation Processes with Very Volatile Components," *AIChE J.*, **32(5)**, 872-874 (1986).
3. R. H. Sherman, J. R. Bartlit and D. K. Veirs, "Experimental Results from Hydrogen/Deuterium Distillations at the Tritium Systems Test Assembly," *Fusion Technol.*, **6(3)**, 625-628 (1984).
4. R. H. Sherman, J. R. Bartlit, K. M. Gruetzmacher, H. Yoshida, T. Yamanishi, T. Naito, S. Hirata, Y. Naruse, "Operation of the TSTA Isotope-Separation System with 100 Gram Tritium," **14(2)**, 1273-1276 (1988).

5. M. Inoue, S. Konishi, T. Yamanishi, S. O'hira, T. Watanabe, K. Okuno, Y. Naruse, R. H. Sherman, J. W. Barnes, J. R. Bartlit, J. L Anderson, "Isotope Separation System Experiments at the TSTA," *Fusion Technol.*, **21(2)**, 293-298 (1992).
6. R. S. Willms, R. H. Sherman, J. B. Riggs, K. Okuno, "Demonstration of Regulatory Process Controls on the TSTA Cryogenic Distillation System," *Fusion Technol.*, **28(3)**, 778-784 (1995).
7. S. Konishi, Y. Yamanishi, M. Enoeda, T. Hayashi, S. O'hira, M. Yamada, T. Suzuki, K. Okuno, R. H. Sherman, R. S. Willms, D. J. Taylor, R. V. Carlson, J. E. Nasise, J. W. Barnes, J. R. Bartlit, J. L. Anderson, "Operation of a Simulated Nonsteady Tokamak Fuel Loop Using the Tritium Systems Test Assembly", *Fusion Engr. And Design*, **28**, 258-264 (1995).
8. R. H. Sherman, D. J. Taylor, T. Yamanisi, M. Enoeda, S. Konishi, K. Okuno, "The Role of Sidestream Recycle in Hydrogen Isotope-Separation and Column Cascade Design," *Fusion Engr. and Design*, **28**, 392-396 (1995).

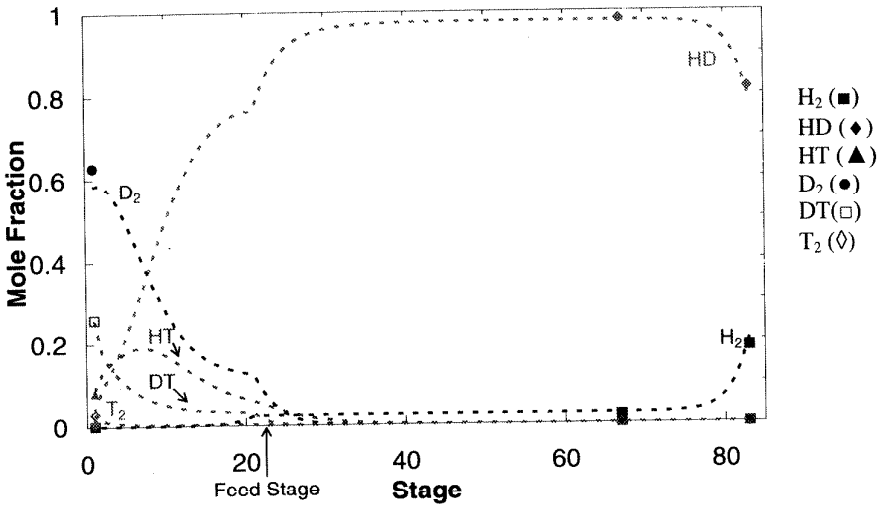

Figure 2:
Case 1
F_{dis}=2500
F_{bot}=5000
Reboiler=34
Feed Stage=21
Inventory=20

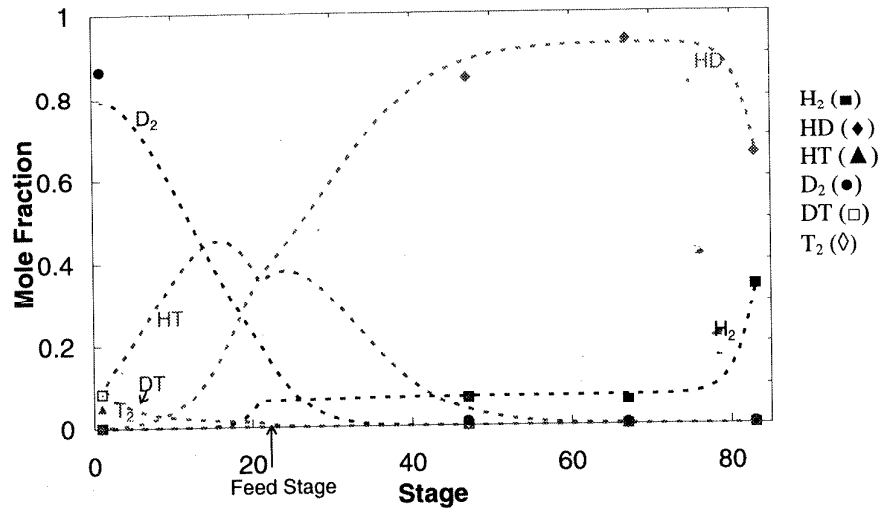

Figure 3:
Case 2
F_{dis}=5000
F_{bot}=2500
Reboiler=34
Feed Stage=21
Inventory=20

Figure 4:
Case 3
F_{dis}=1000
F_{bot}=2000
Reboiler=36
Feed Stage=21
Inventory=20

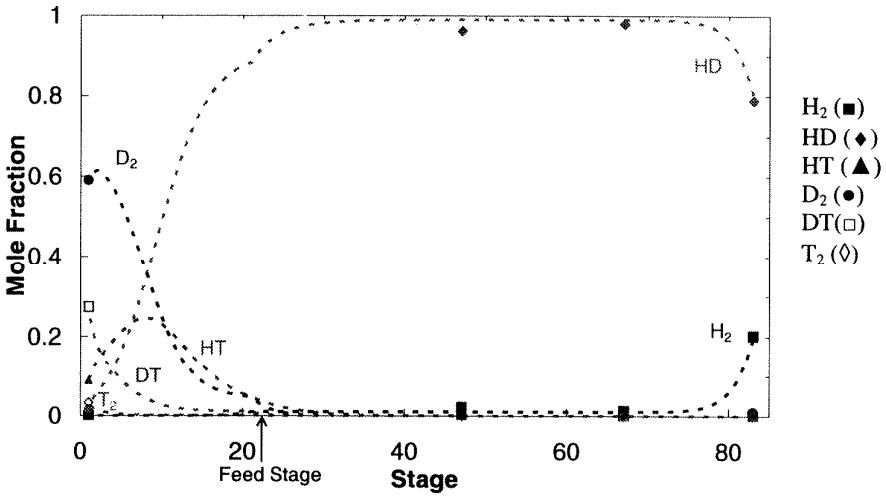

Figure 5:
Case 4
F_{dis}=1000
F_{bot}=2000
Reboiler=18
Feed Stage=47
Inventory=15

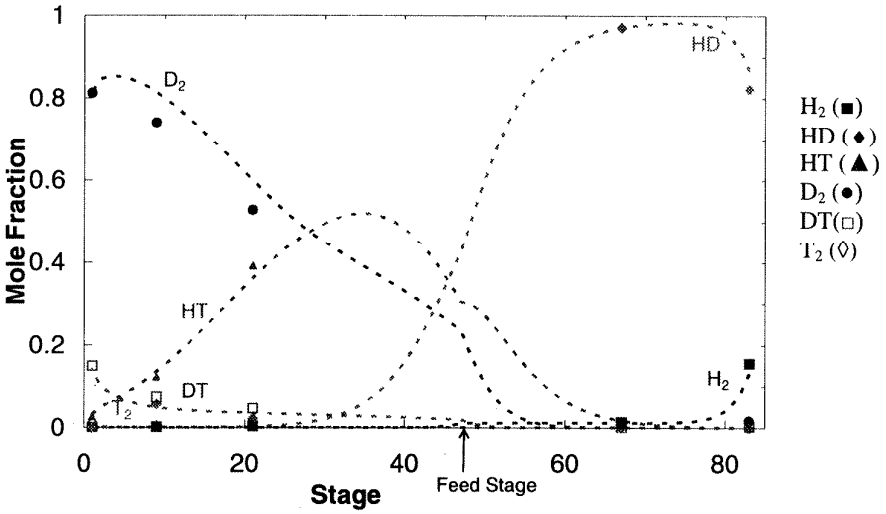

Figure 6:
Case 5
F_{dis}=2000
F_{bot}=2000
Reboiler=18
Feed Stage=47
Inventory=15

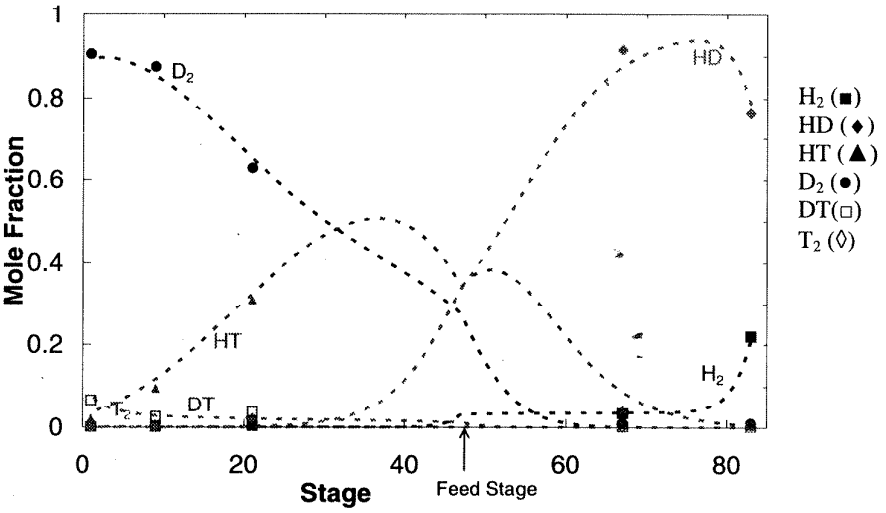

Table 1: Process Conditions for Each Case

Case	1	2	3	4	5
Distillate Flowrate, sccm	2500	5000	1000	1000	2000
Bottoms Flowrate, sccm	5000	2500	2000	2000	2000
Top Temperature, K	22.3	22.3	22.2	22.4	22.6
Bottom Temperature, K	24.4	24.4	24.4	24.6	24.9
Pressure, torr	850	863	862	860	933
Reboiler Duty, W	34.3	34.3	36.2	17.8	17.6
Liquid Level, mm	46	46	42	16	18
Inventory, Diatomic Moles	19.9	19.9	19.9	14.8	14.8

Table 2: Measured Hydrogen Isotope Compositions for Each Case

	Measured Species Mole Fraction					
Stage	**H_2**	**HD**	**HT**	**D_2**	**DT**	**T_2**
Case 1						
83	0.184	0.816	0.000	0.000	0.000	0.000
67	0.019	0.981	0.000	0.000	0.000	0.000
21*	0.063	0.283	0.053	0.413	0.170	0.017
1	0.000	0.007	0.079	0.628	0.257	0.029
Case 2						
83	0.339	0.657	0.000	0.004	0.000	0.000
67	0.061	0.935	0.000	0.004	0.000	0.000
47	0.071	0.846	0.073	0.010	0.000	0.000
21*	0.235	0.444	0.020	0.274	0.027	0.000
1	0.000	0.000	0.048	0.865	0.087	0.000
Case 3						
83	0.203	0.788	0.000	0.009	0.000	0.000
67	0.013	0.979	0.003	0.004	0.000	0.000
47	0.022	0.962	0.002	0.009	0.004	0.000
21*	0.069	0.295	0.058	0.383	0.172	0.023
1	0.000	0.017	0.088	0.590	0.273	0.032
Case 4						
83	0.156	0.823	0.000	0.017	0.004	0.000
67	0.014	0.971	0.005	0.009	0.000	0.000
47*	0.049	0.278	0.023	0.552	0.092	0.006
21	0.004	0.021	0.391	0.529	0.047	0.007
9	0.002	0.057	0.122	0.740	0.074	0.005
1	0.000	0.000	0.026	0.812	0.149	0.013
Case 5						
83	0.220	0.762	0.003	0.010	0.000	0.005
67	0.034	0.915	0.043	0.008	0.000	0.000
47*	0.115	0.402	0.015	0.433	0.032	0.003
21	0.004	0.022	0.307	0.627	0.037	0.003
9	0.000	0.005	0.095	0.874	0.026	0.000
1	0.000	0.000	0.020	0.905	0.068	0.007

* Feed Stage