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Nuclear Waste Treatment Program

**MASBAL: A Computer
Program for Predicting the
Composition of Nuclear
Waste Glass Produced by a
Slurry-Fed Ceramic Melter**

P. W. Reimus

July 1987

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
Operated for the U.S. Department of Energy
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PACIFIC NORTHWEST LABORATORY
operated by
BATTELLE MEMORIAL INSTITUTE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC06-76RLO 1830

Printed in the United States of America
Available from
National Technical Information Service
United States Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

NTIS Price Codes
Microfiche A01

Printed Copy

Pages	Price Codes
001-025	A02
026-050	A03
051-075	A04
076-100	A05
101-125	A06
126-150	A07
151-175	A08
176-200	A09
201-225	A010
226-250	A011
251-275	A012
276-300	A013

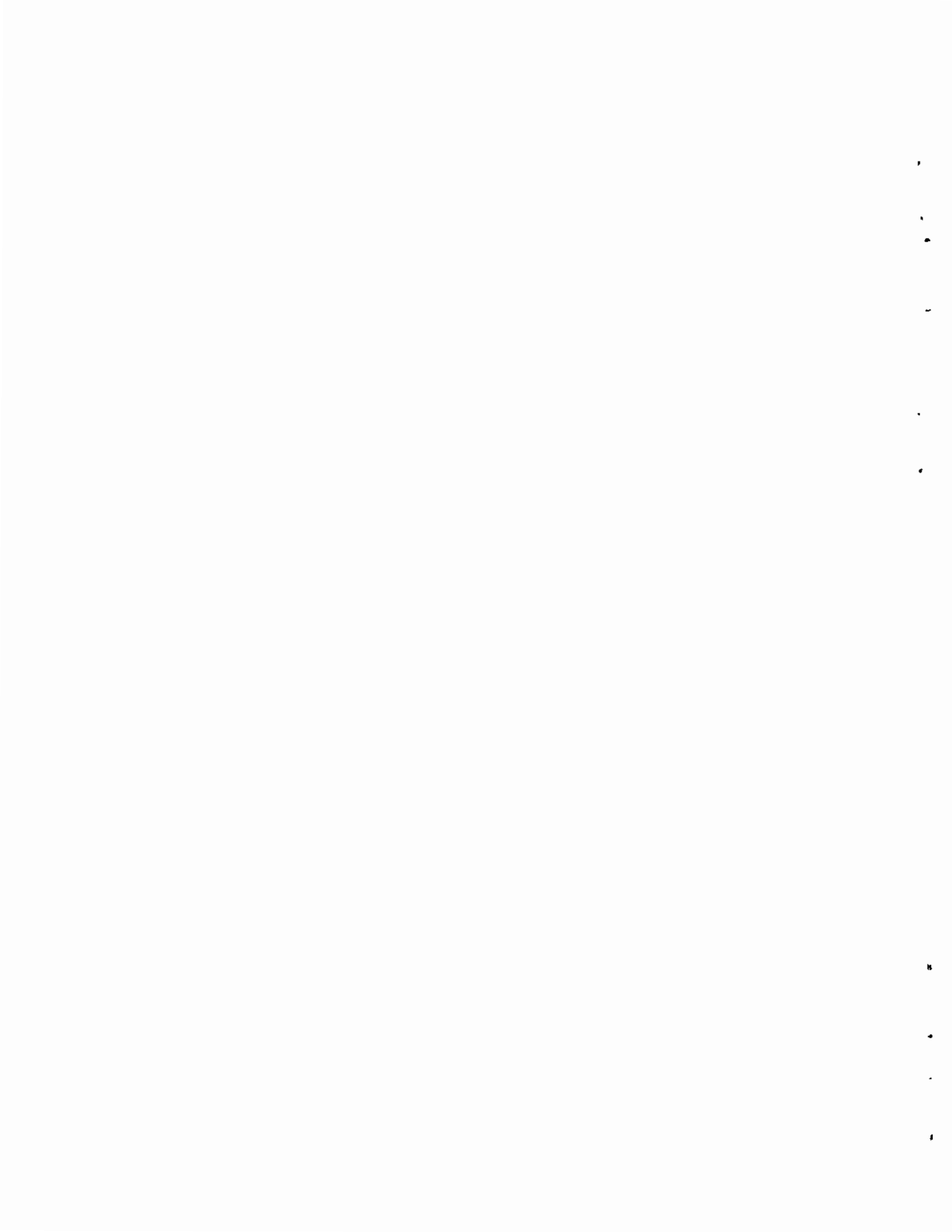
MASBAL: A COMPUTER PROGRAM FOR PREDICTING THE
COMPOSITION OF NUCLEAR WASTE GLASS PRODUCED BY
A SLURRY-FED CERAMIC MELTER

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Richland, Washington 99352



SUMMARY

This report serves as a user's manual for the MASBAL computer program. MASBAL has three overall objectives: 1) to predict the composition of nuclear waste glass produced by a slurry-fed ceramic melter based on a knowledge of process conditions; 2) to generate simulated data that can be used to estimate the uncertainty in the predicted glass composition as a function of process uncertainties; and 3) to generate simulated data that can be used to provide a measure of the inherent variability in the glass composition as a function of the inherent variability in the feed composition. These three capabilities are important to nuclear waste glass producers because there are constraints on the range of compositions that can be processed in a ceramic melter and on the range of compositions that will be acceptable for disposal in a geologic repository.

MASBAL was developed specifically to simulate the operation of the West Valley Component Test System, a commercial-scale ceramic melter system that will process high-level nuclear wastes currently stored in underground tanks at the site of the Western New York Nuclear Services Center (near West Valley, New York). The program is flexible enough, however, to simulate any slurry-fed ceramic melter system.

MASBAL simulates the flow of material through the melter feed tank and melter of the vitrification system. The program can track as many as 100 constituents through the system. These constituents are assumed to be inert at all points in the system (i.e., concentrations are specified on an oxide basis). Material enters the system by way of the feed tank (slurry transfer from the makeup tank), and it leaves the system by going out either the off-gas system or into a canister. MASBAL can simulate the addition of glass-forming compounds directly to either the feed tank or the melter (these actions may be taken if the feed or glass composition deviates significantly from the target composition). The off-gas system is modeled as a sink for components that have finite melter decontamination factors. The primary outputs of MASBAL are the composition of the glass exiting the melter as a function of time and the average composition of the glass in each glass pour.

Because the mixing characteristics of the West Valley melter are currently unknown, MASBAL provides several options for modeling flow of material through the melter. The melter can be modeled as 1) a single ideally-mixed tank, 2) two to five ideally-mixed regions in series, or 3) a plug flow region followed by one or two ideally-mixed regions in series. The best modeling approach will be decided by the best fit to experimental data. The relative volumes of each region are adjustable for use in calibration/validation activities.

MASBAL is designed to be operated in three modes. The first mode provides deterministic predictions of the glass composition exiting the melter as a function of time. The key inputs to the program when it is operated in this mode are the values of process measurements taken at appropriate times during the operation of the system (i.e., actual process data).

The second mode generates simulated glass composition data that can be used to estimate the uncertainty in the deterministic predictions provided by the first mode. The process data required as inputs for the first mode are also required for the second mode. The parameters of statistical distributions that define uncertainties in the process measurements are also required as inputs for the second mode. Each process measurement is treated as the mean or mode of a statistical distribution that is assumed to contain the true value of the variable being measured. Measurement errors are simulated by randomly sampling these distributions; the values returned from the distributions are used in subsequent mass balance calculations as the true values of the measured variables. MASBAL can be run repeatedly in this mode to generate glass composition data that are distributed randomly about the deterministic predictions of mode 1. The absolute differences between the data generated in mode 2 and the predictions of mode 1 provide a measure of the uncertainty in the deterministic predictions.

When MASBAL is run in the third mode, the program generates its own feed composition data by randomly selecting the composition of successive batches of feed from statistical distributions defined by the user (the concentration of each constituent in the feed will be taken from a distribution that has a mean or mode of the target concentration). All process measurements are simulated

by randomly sampling statistical distributions that have means or modes equal to the simulated values of the process variables being measured. The simulated fluctuations in the feed composition and errors in process measurements cause the calculated glass composition to fluctuate randomly about the target composition. If the process measurements are treated deterministically (i.e., if the standard deviations describing the measurement errors are set to zero), then the absolute differences between the stochastically generated data and the target glass composition will provide a measure of the inherent variability in the composition of the glass as a function of the variability in the feed composition. If, on the other hand, the composition of successive batches of feed is treated deterministically, then the differences between the stochastically generated composition data and the target glass composition will provide the same information that is provided by the second mode of MASBAL. The advantage of running MASBAL in the third mode is that the user can run the program without having to supply process data (all that is required are the parameters of distributions that describe feed composition variability and uncertainties in process measurements). This feature gives MASBAL the capability to simulate thousands of hours of operation of the melter system, and thus makes it possible to generate enough simulated data to make reasonable estimates of the confidence limits associated with either the predicted or the target glass composition.

MASBAL consists of PNL-developed FORTRAN subroutines that are integrated with the SIMAN simulation language. SIMAN offers 1) a differential equation solving algorithm for solving the mass balance differential equations that describe the time dependent concentrations in the system, 2) the capability to model discrete events that interact with or change the values of state variables in the system (e.g., the starting or stopping of the flow of feed to the melter, and 3) the capability to randomly sample statistical distributions. The random sampling of statistical distributions is an essential feature of MASBAL when it is operated in modes 2 or 3.

This report provides a complete description of the features of MASBAL. Each of the input and output files is thoroughly described, and instructions on how to run the program are provided. Examples of each of the input and output files are included in appendices.

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1.0 INTRODUCTION

This report serves as a user's manual for the MASBAL computer program. MASBAL has three primary objectives: 1) to predict the composition of nuclear waste glass produced by a slurry-fed ceramic melter based on a knowledge of process conditions, 2) to generate simulated data that can be used to estimate the uncertainty in the predicted glass composition as a function of process uncertainties, and 3) to generate simulated data that can be used to provide a measure of the inherent variability in the glass composition as a function of the inherent variability in the feed composition.

MASBAL was developed at Pacific Northwest Laboratory (PNL)^(a) for West Valley Nuclear Services (WVNS) Company, Inc. WVNS is responsible for management of the site of the Western New York Nuclear Services Center, the only commercial nuclear fuel reprocessing plant to have operated in the United States. Underground tanks at the site contain high-level waste (HLW) produced in part by a commercial fuel reprocessing campaign. The State of New York has assumed responsibility for these wastes. The U.S. Department of Energy (DOE) is assisting, through the West Valley Demonstration Project (WVDP), in the retrieval and solidification of these wastes.

The planned method of solidification of the HLW is incorporation into a vitreous glass matrix. The waste slurry from the storage tanks will be combined with appropriate glass-forming compounds, concentrated, and then fed to a ceramic melter operated at 1100° to 1250°C. Water from the slurry will be driven off immediately, and the remaining components will gradually melt into a molten glass phase in the melter. Glass will be poured from the melter into canisters, where it will cool and solidify. The canisters will eventually be sealed and shipped to a high-level nuclear waste repository for disposal.

The ability to predict the glass composition in the canisters and the uncertainty in the glass composition is important for two reasons: 1) there are constraints on the range of compositions that can be processed in a ceramic

(a) Operated for the U.S. Department of Energy by Battelle Memorial Institute.

melter, and 2) there are constraints on the range of compositions that will be acceptable for disposal in a geologic repository.

The first set of constraints arises because the composition of the glass affects key processing parameters such as the melting point, melting rate, viscosity, electrical conductivity of the mixture, and the tendency of the mixture to foam. The second constraint arises because composition is an important parameter affecting the durability of the glass to aqueous attack, one of the key measures of the acceptability of any waste form for geologic disposal. Because of the dependence of durability on composition, WVNS will probably be required to provide the DOE Office of Civilian Radioactive Waste Management (OCRWM) or perhaps a regulatory agency with an estimate of the composition of the glass in each canister that is produced.

MASBAL provides WVNS with the capability to predict the composition of the glass in each canister based on process measurements taken upstream of the canisters. It also provides

- the capability to estimate the uncertainty in the predicted glass composition as a function of 1) uncertainties in process measurements, and 2) the number of replicate feed samples taken and the number of replicate analyses performed on each sample
- the capability to estimate the variability in the actual glass composition as a function of the inherent variability in the feed composition.

Chapter 2.0 of this report provides a detailed description of the design of MASBAL. The input files and the input data that they contain are discussed in Chapter 3.0. Because the input files represent the only interface between the user and the program, Chapter 3.0 is extremely important to the user. A description of the output files is provided in Chapter 4.0. Chapter 5.0 provides instructions on how to execute MASBAL. Results from some of the test cases that were run during the development of MASBAL are presented in Chapter 6.0. These test cases illustrate some of the capabilities of the program. Examples of input and output files are provided in Appendices A and B, respectively.

2.0 SOFTWARE DESIGN

MASBAL is a computer program that simulates the operation of a slurry-fed ceramic melter system. The primary inputs to the program are 1) the design parameters of the melter system, 2) the process measurements taken during operation of the system, and 3) the parameters of statistical distributions that describe uncertainties in the process measurements and inherent fluctuations in the feed composition. The primary output of the program is the calculated glass composition exiting the melter as a function of time.

2.1 DESCRIPTION OF THE PHYSICAL SYSTEM

A schematic drawing of the West Valley Component Test System (CTS) is shown in Figure 2.1. The following operating scenario was assumed for the purposes of the simulation:^(a) During a vitrification campaign, waste slurry is pumped from the high-level waste feed tank to the concentrator feed makeup tank, where it is sampled. The apparent composition of the samples is used to calculate the amount of various glass forming compounds that should be added to the waste to obtain a slurry of the desired feed composition. These chemicals are added first to a cold chemical makeup tank, where they are blended. They are then transferred to the concentrator feed makeup tank, where they are combined with the waste. After addition of the glass formers, the slurry in the makeup tank is concentrated until the solids loading is at some specified level. The slurry is then transferred to the feed tank, where it is continuously fed to the melter. When the slurry enters the melter, the water quickly evaporates and goes to the off-gas system, leaving the less volatile constituents behind to gradually melt into the molten glass phase. Small amounts of each of these less volatile constituents will go to the off-gas system as a result of being entrained in the exiting gases or because of partial volatilization in the melter. The purpose of the off-gas system is to remove the radioactive constituents from the gas so that the gas can be exhausted to the environment. Glass is poured out of the melter either continuously or in batches into metal canisters.

(a) This operating strategy reflects current plans at West Valley.

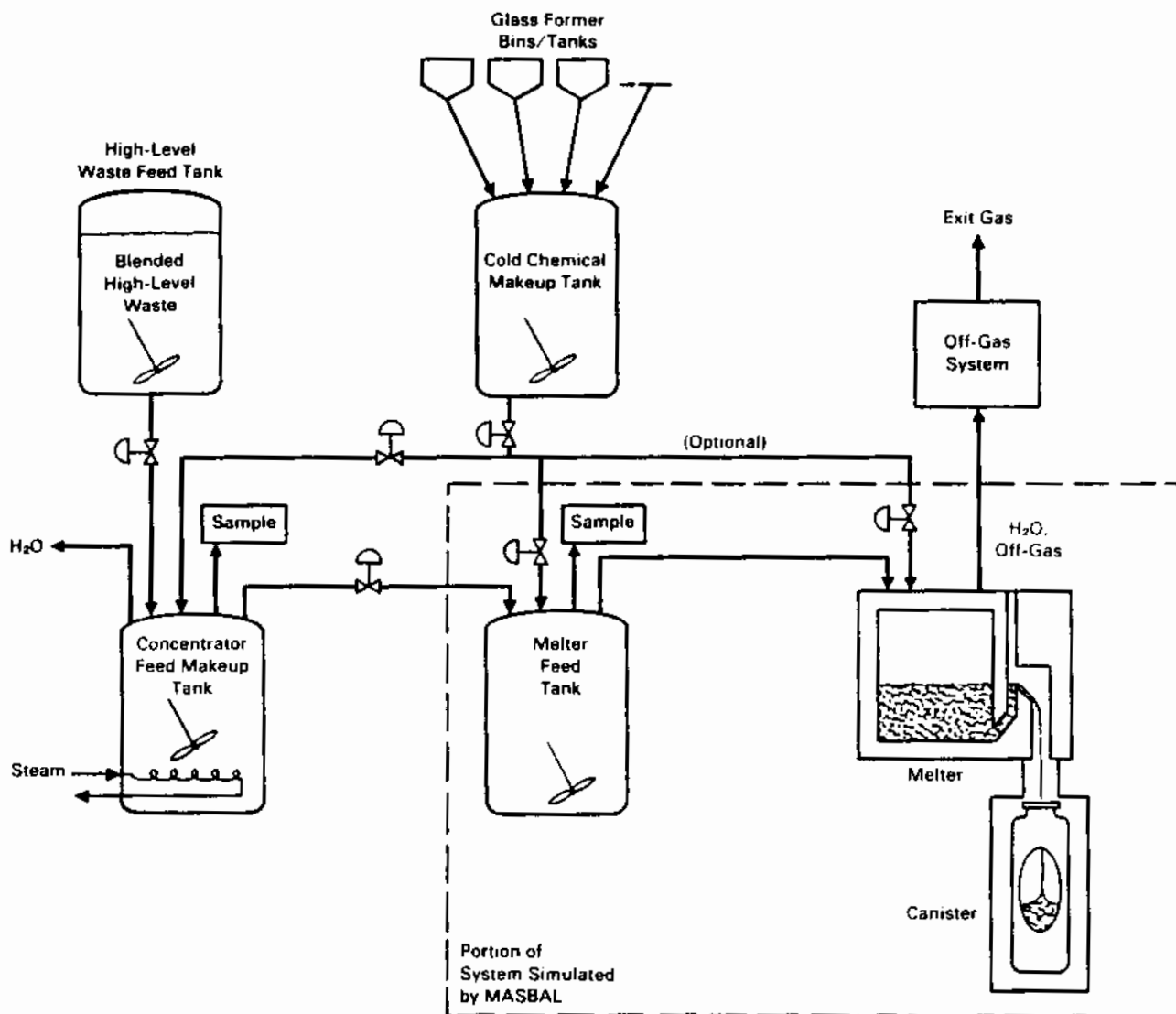


FIGURE 2.1. West Valley Component Test System Schematic

MASBAL simulates only the part of the system that is contained within the dashed line in Figure 2.1. The makeup tank is excluded because WVNS plans to sample the feed tank after each transfer of slurry from the makeup tank. Therefore, the glass compositions calculated by MASBAL are based on the analyses of samples from the feed tank rather than from the makeup tank.

The slurry lines that run from the cold chemical makeup tank to the feed tank and melter in Figure 2.1 could be used to add glass formers directly to the latter two tanks. This action might be taken if a sample from the feed tank indicates that the feed composition is out of tolerance and must be

corrected. The West Valley CTS currently does not have a line running from the cold chemical makeup tank to the melter, but such a line is included in MASBAL for completeness.

The off-gas system is excluded from MASBAL because the objective of MASBAL is to calculate the composition of the glass poured into the canisters, not the composition in the off-gas system. However, the amount of each constituent that is collected in the off-gas system is a necessary input to MASBAL because the composition of the glass is calculated by differencing between the feed composition and the off-gas composition.

2.2 ASSUMPTIONS AND BASES

MASBAL was developed under the following set of assumptions and bases:

- The model includes a provision for as many as 100 chemical constituents.
- The model assumes that all chemical constituents are inert at all points in the system (chemical reactions are not modeled). The concentration of each chemical constituent is specified as a mass of oxide (or other final glass form) per unit volume. Each constituent that appears in the glass is treated as a separate inert component. Water is the only component that does not appear in the glass.
- The main feed tank is modeled as an ideally-mixed tank. Based on studies at PNL, this assumption should be valid if sufficient power is supplied to the tank in the form of agitation (Peterson et al. 1986).
- The melter can be modeled as an ideally-mixed tank, as a plug flow region followed by one or two ideally-mixed regions in series, or as two to five ideally-mixed regions in series.
- There is no holdup in lines between tanks (i.e., the volume of slurry in pipes is negligible compared to the volume in tanks).
- The rate of volatilization of constituents in the melter is modeled as constant from one off-gas sampling time to another. No attempt is made to model off-gas surges or fluctuations. If the off-gas is not

sampled or if no sampling information is available, losses due to volatilization are modeled using a constant decontamination factor for each constituent.

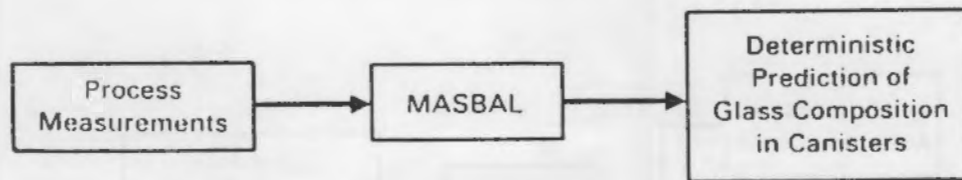
- Batch glass pours are modeled as having a constant flow rate for a specified time period.

2.3 MODES OF OPERATION

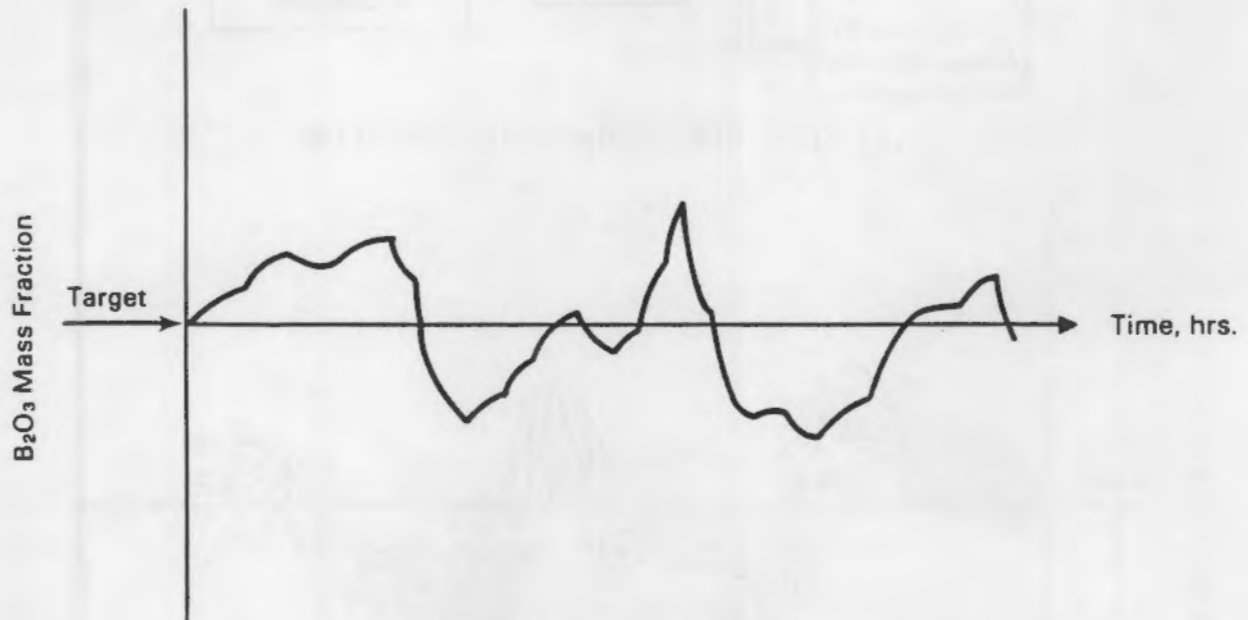
MASBAL is designed to be operated in three modes. The first mode provides deterministic predictions of the glass composition as a function of time. The second and third modes generate simulated glass composition data that can be used to estimate the uncertainty in the deterministic predictions provided in mode 1, or to estimate the variability in the glass composition as a function of the inherent variability in the feed composition.

When MASBAL is operated in the first mode, the key program inputs are process measurements and control actions taken at appropriate times during the operation of the system. The program takes these inputs and simulates the system deterministically to calculate the composition of the glass exiting the melter as a function of time. The operation of the program in this mode is depicted in Figure 2.2a. A typical plot of output from mode 1 is provided in Figure 2.2b, which shows the predicted mass fraction of B_2O_3 in the glass as a function of time. The fluctuations in the glass composition are primarily a result of fluctuations in the measured feed composition, which are input to the program. Figure 2.2b does not represent actual output from a MASBAL run; it is simply a schematic drawing showing how the output from mode 1 is expected to look.

In the second mode, the key inputs to MASBAL are the parameters of statistical distributions that define uncertainties in process measurements. The inputs used in the first mode are also required as inputs in the second mode, but they are now used as the "most likely" values of distributions rather than as deterministic values. A statistical distribution is randomly sampled each time there is a process measurement. The value returned from the distribution is treated as the "true" or actual value of the measurement. Because the returned value is usually different from the "most likely" value, this



(a) Block Diagram Depicting Operation

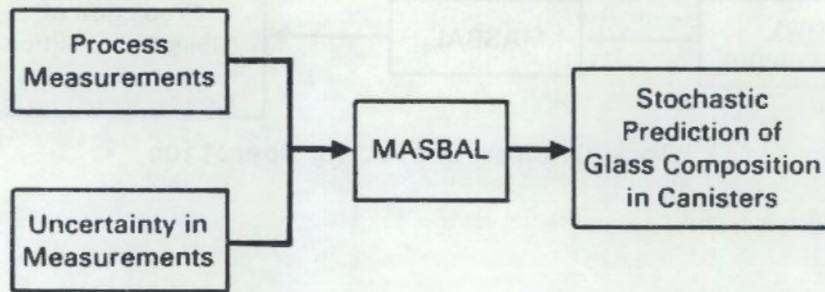


(b) Typical Plot of Output

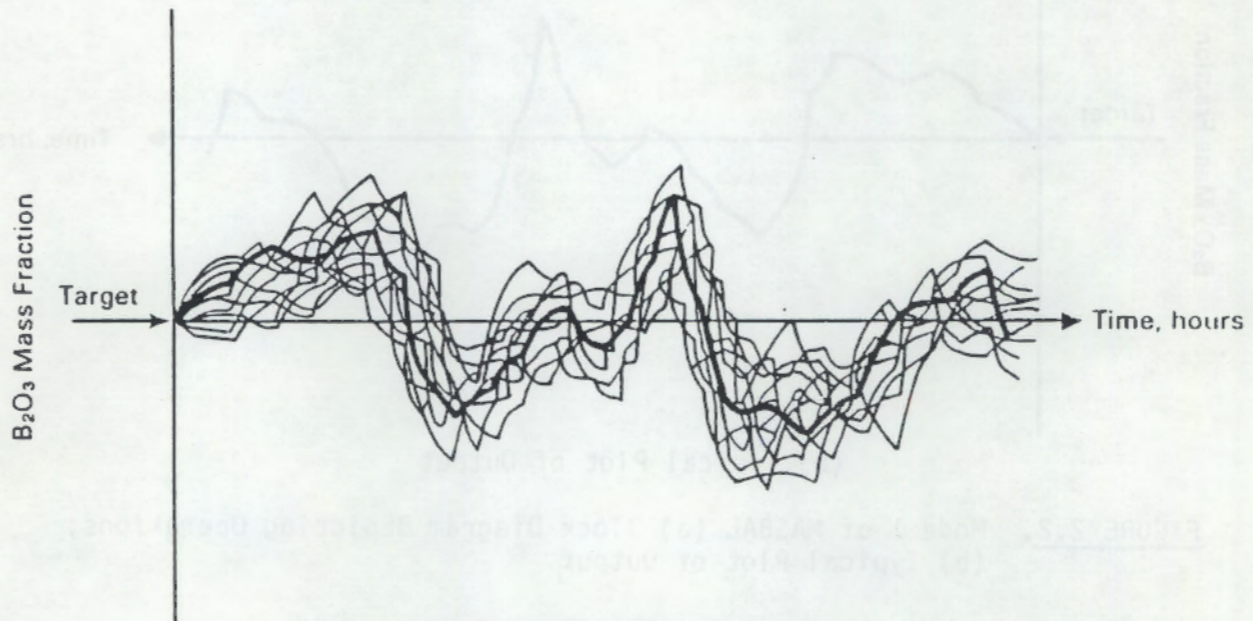
FIGURE 2.2. Mode 1 of MASBAL (a) Block Diagram Depicting Operations; (b) Typical Plot of Output

procedure simulates errors in the process measurements. If a number of runs are performed using the same set of inputs (with a different random number stream for each run), a population of simulated glass compositions that are randomly distributed about the deterministic composition calculated in mode 1 will be obtained.

A block diagram depicting the operation of MASBAL in mode 2 and a typical plot showing output from mode 2 are provided in Figure 2.3. Each of the light solid lines in Figure 2.3b represents the output from one run in mode 2. The dark solid line represents the output from mode 1. It appears that the output from mode 2 forms an envelope about the mode 1 predictions. The width of this envelope provides a qualitative measure of the uncertainty associated with the composition predicted in mode 1. The absolute differences between the glass



(a) Block Diagram Depicting Operation



(b) Typical Plot of Output

FIGURE 2.3. Mode 2 of MASBAL (a) Block Diagram Depicting Operation; (b) Typical Plot of Output

compositions calculated in modes 2 and 1 can be used to construct confidence intervals about the mode 1 predictions, which provide a quantitative measure of the uncertainty in the deterministic predictions.

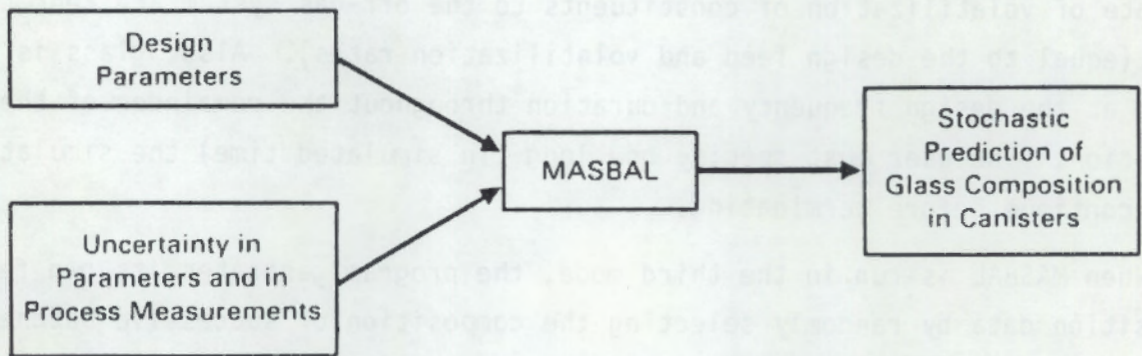
When MASBAL is run in the first or second mode, the simulation is driven by process data that are provided as input to the program. These data include information on what has happened in the system prior to the current time, but they contain no information about future events. Because it may be of interest to predict the composition of the glass that will be poured in the next several canisters (based on the current composition in the feed tank and melter),

MASBAL continues to simulate the system by generating its own data for future process data. The user is given two options for continuing execution of the program: 1) all batches of feed following the last batch will be given the target composition, or 2) the next N batches of feed will be given the same composition as the last batch, where N is specified by the user. When MASBAL is run in mode 1, the compositions of succeeding feed batches are deterministic. When the program is run in mode 2, the compositions are stochastic, and the mean composition is either the target composition or the composition of the most recent batch, depending on the option selected. The melter feed rate and the rate of volatilization of constituents to the off-gas system are kept constant (equal to the design feed and volatilization rates). Also, glass is poured at the design frequency and duration throughout the remainder of the simulation. The user must specify how long (in simulated time) the simulation is to continue before terminating.

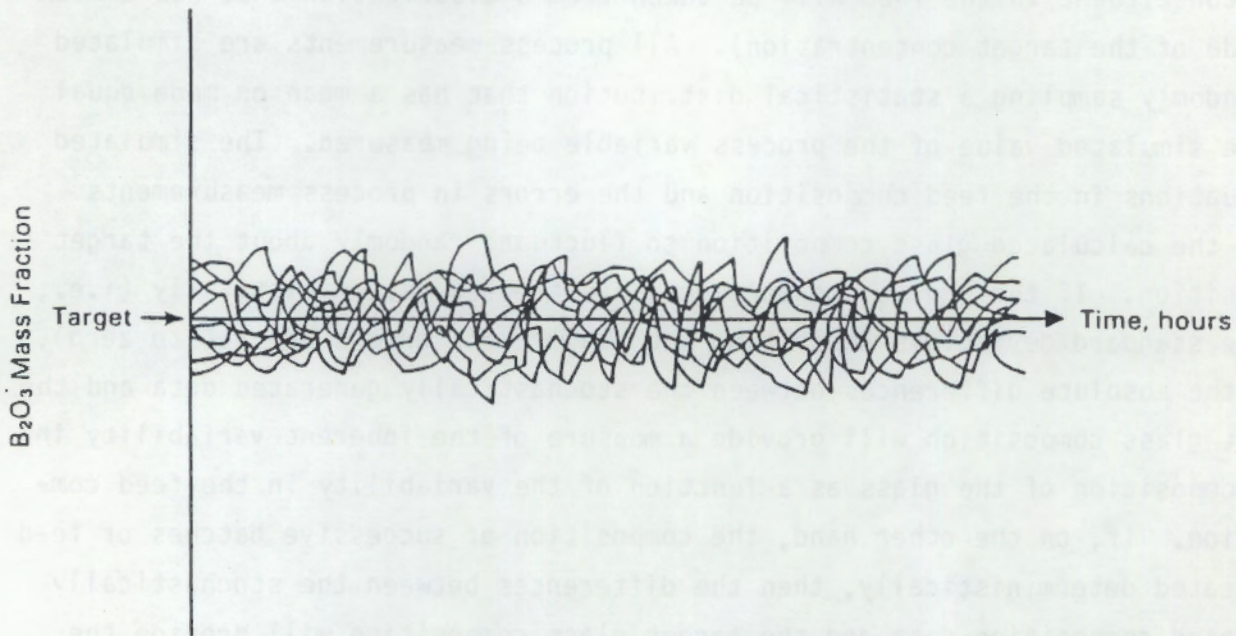
When MASBAL is run in the third mode, the program generates its own feed composition data by randomly selecting the composition of successive batches of feed from statistical distributions defined by the user (the concentration of each constituent in the feed will be taken from a distribution that has a mean or mode of the target concentration). All process measurements are simulated by randomly sampling a statistical distribution that has a mean or mode equal to the simulated value of the process variable being measured. The simulated fluctuations in the feed composition and the errors in process measurements cause the calculated glass composition to fluctuate randomly about the target composition. If the process measurements are treated deterministically (i.e., if the standard deviations describing the measurement errors are set to zero), then the absolute differences between the stochastically generated data and the target glass composition will provide a measure of the inherent variability in the composition of the glass as a function of the variability in the feed composition. If, on the other hand, the composition of successive batches of feed is treated deterministically, then the differences between the stochastically generated composition data and the target glass composition will provide the same information that is provided by the second mode of MASBAL. The advantage of running MASBAL in the third mode is that the user can run the program without having to supply process data; only the parameters of distributions that

describe feed composition variability and uncertainties in process measurements are required. This feature gives MASBAL the capability to simulate thousands of hours of operation of the melter system, and thus makes it possible to generate enough simulated data to make reasonable estimates of the confidence limits associated with either the predicted or the target glass composition.

A block diagram depicting the operation of MASBAL in mode 3 and a typical plot of output from mode 3 are shown in Figure 2.4. Each of the lines in Figure 2.4b represents the output from one run in mode 3. The straight,



(a) Block Diagram Depicting Operation



(b) Typical Plot of Output

FIGURE 2.4. Mode 3 of MASBAL (a) Block Diagram Depicting Operation; (b) Typical Plot of Output

horizontal line represents the target composition. The output is very similar to the output from mode 2, except that the glass composition fluctuates about the target composition rather than the composition calculated by mode 1.

2.4 MASS BALANCE EQUATIONS

The key equations in MASBAL are the differential and state equations that describe the change of mass with time of each constituent in the feed tank, melter, and canisters. The feed tank in MASBAL is modeled as an ideally-mixed tank. The user is given the option of modeling the melter in one of three ways:

1. as an ideally-mixed tank
2. as a combination of one plug flow and up to two ideally-mixed regions in series - The plug flow region is the first region in the series, followed by the smaller of the two ideally-mixed regions (if there are two). The user must specify the percentage of melter volume that is plug flow and the percentage that constitutes each of the ideally-mixed regions. These percentages will apply when the melter is operated at steady state.
3. as two to five ideally-mixed regions in series - The user must specify the volume percentages of each of the regions at steady state.

Each glass pour into a canister is treated as a pour into an ideally-mixed tank that has no outlet stream.

2.4.1 Mass Balance Equations for Ideally-Mixed Regions

The overall mass balance equation around an ideally-mixed region is given by

$$dW/dt = Q_f - Q_p \quad (2.1)$$

where W = mass or volume of the ideally-mixed region, kg or L

t = time, hr

Q_f = flow rate into region, kg/hr or L/hr

Q_p = flow rate into region, kg/hr or L/hr

The equation describing the change in mass over time of an individual constituent in an ideally-mixed region is

$$d(M_i)/dt = Q_f * X_{if} - Q_p * X_{ip} \quad (2.2)$$

where M_i = mass of constituent i in the ideally-mixed region, kg

X_{if} = concentration of constituent i in inlet stream, mass fraction or kg/L

X_{ip} = concentration of constituent i in outlet stream, mass fraction or kg/L.

By convention, concentrations in the aqueous feed slurry are generally expressed as kg oxide/L, while concentrations in the molten glass are generally expressed as mass fractions. Equations (2.1) and (2.2) also hold for individual glass pours into canisters, except that Q_p for these "regions" is zero.

The instantaneous concentration or mass fraction of a constituent in an ideally-mixed region is given by

$$X_{ip} = M_i/W \quad (2.3)$$

Because ideal mixing implies that the concentration at every point in the region is the same, X_{ip} is also the concentration in any stream that exits the ideally-mixed region.

2.4.2 Mass Balance Equations for Plug Flow Region in Melter

By definition, all elements of mass in the plug flow region must exit in the same order that they entered (i.e., there is no mixing). The cumulative mass that enters the plug flow region and the cumulative mass that exits the region are both continuously monitored by MASBAL. The program periodically records the composition of mass elements that enter the region. The composition of a mass element exiting the region is then set equal to the composition of a mass element that entered the region at the time when the total cumulative

mass having entered the region (minus the initial mass) was equal to the total cumulative mass that has now exited the region. This situation is expressed mathematically as

$$X_{ioZ} = X_{if}(Z - Z_i) \quad (2.4)$$

where X_{ioZ} = mass fraction of constituent i in a mass element exiting the region after Z kg of cumulative mass have exited the region
 $X_{if}(Z - Z_i)$ = mass fraction of constituent i in a mass element entering the region after $(Z - Z_i)$ kg of cumulative mass have entered the region

Z_i = initial mass in plug flow region, kg.

The composition of mass elements entering the plug flow region are updated once each hour of simulated time or whenever the concentration of a constituent in the inlet stream changes by 1% (to adequately model the plug flow region when the composition is changing rapidly). The composition of a mass element that enters the region between two consecutive updating times is calculated by linear interpolation of the compositions recorded at the two times.

2.4.3 Changes in Mass of Melter Regions as a Function of Feed Rate

When the melter is not modeled as a single ideally-mixed region, the user must specify the percentage of the total mass that is allocated to each region (the inputs are actually entered as volume percentages). MASBAL assumes that these percentages are valid only when the feed rate is equal to the design feed rate. If the feed rate drops below the design feed rate, the mass of all regions except the last region will drop proportionately (i.e., a 10% drop in feed rate will result in a 10% drop in these volumes). The rate at which the mass changes is modeled as an exponential decay with a time constant proportional to the steady-state mass in the melter divided by the design feed rate (in kg oxides/hr). The last two sentences are expressed mathematically in Equations (2.5) through (2.7).

$$Q_i = Q_d * W_i / W_d \quad (2.5)$$

$$W_f = W_d * Q_f / Q_d \quad (2.6)$$

$$dW/dt = -(Q_i - Q_f) * \beta W_d / W_s * \exp(-t / (W_s / \beta Q_d)) \quad (2.7)$$

where Q_i = equivalent feed rate before change in feed rate, kg oxides/hr
 Q_f = new feed rate, kg oxides/hr
 Q_d = design feed rate, kg oxides/hr
 W_i = instantaneous mass of region before change in feed rate, kg
 W_f = steady-state mass of region at new feed rate, kg
 W_d = steady-state mass of region at design feed rate, kg
 β = user-specified parameter for adjustment of time constant
 W_s = steady-state mass of all regions in melter at the design feed rate, kg
 W = instantaneous mass of region, kg
 t = time since change in feed rate occurred, hr.

The integrated form of Equation (2.7), which gives the actual mass of melter regions (other than the last region) as a function of time after a change in feed rate, is

$$W = W_i - W_d(Q_i - Q_f) / Q_d * [1 - \exp(-t(W_s / \beta Q_d))] \quad (2.8)$$

Equations (2.7) and (2.8) work well when the feed rate is within a factor of two or three of the design feed rate, but they tend to overpredict the increase in mass of the region(s) whenever the feed rate is more than an order of magnitude greater than the design feed rate. This situation can physically arise when glass formers are added directly to the melter from the cold chemical makeup tank, because the transfer of slurry can be very rapid. In this case, the equation used to calculate the change in mass of all regions (except the last region) in the melter is

$$dW/dt = -(Q_i - Q_f) / (N - 1) * \exp[-t / ((N-1) W_d / Q_d)] \quad (2.9)$$

where N is the number of regions in the melter.

The integrated form of Equation (2.9) is

$$W = W_i - W_d(Q_i - Q_f)/Q_d * [1 - \exp[-t/((N-1) W_d/Q_d)]] \quad (2.10)$$

Equations (2.9) and (2.10) are used to describe the change in mass of all melter regions (except the last region) whenever glass formers are being added directly to the melter.

The change in mass of the last region in the melter is determined from a mass balance around the last region:

$$dW_L/dt = Q_f - \sum_{j=1}^{N-1} dW_j/dt - P \quad (2.11)$$

where W_L = mass of last region in melter, kg

W_j = mass of j th region in melter, kg

N = total number of regions in melter

P = pouring rate of glass into canister, kg/hr.

Equation (2.11) ensures that the mass balance around the entire melter remains as

$$dW_t/dt = Q_f - P \quad (2.12)$$

where W_t is the total mass of glass (kg) in the melter

The approach outlined above ensures that when the feed rate, Q_f , is zero (i.e., the melter is idling), the melter will approach an ideally-mixed state rather than remain in a non-ideal state. This situation is believed to be realistic for idling melters. When the feed rate increases, the volume of all regions except the last region will increase proportionately and at an

exponential rate.^(a) If the time-averaged glass pouring rate is increased along with the feed rate (as it should be unless it is desired to raise the level of glass in the melter), the last region in the melter will decrease in mass at a rate equal to the sum of the rates of increase for the other regions.

2.4.4 Off-Gas Calculations

Losses to the off-gas system are modeled by splitting the melter inlet stream into two streams, one going directly to the off-gas system and the other going to the first region in the melter. Assuming that the off-gas has been sampled and that information is available regarding the mass of each constituent that has been collected in the off-gas system (over a certain period of time), the following equations apply:

$$Q_{io} = M_{io}/t \quad (2.13)$$

$$Q_{if} = Q_e * x_{ie} - Q_{io} \quad (2.14)$$

$$Q_o = \sum_{i=1}^N Q_{io} \quad (2.15)$$

$$Q_f = \sum_{i=1}^N Q_{if} \quad (2.16)$$

(a) It should be recognized that as the feed rate is increased or decreased, the power to the melter is generally increased or decreased. Because an increase in power generally increases the amount of natural convection in the melter (and vice-versa), the volume of the plug flow and smaller well-mixed regions may not necessarily change in proportion to the feed rate. However, until data become available that suggest otherwise, the plug flow and smaller well-mixed regions will be modeled as stated above.

where Q_{io} = flow rate of constituent i into off-gas system, kg oxide/hr
 M_{io} = mass of constituent i collected in off-gas system, kg
 t = time duration over which mass M_{io} was collected, hr
 Q_{if} = flow rate of constituent i into 1st melter region, kg oxide/hr
 Q_e = total flow rate entering melter, kg oxide/hr
 X_{ie} = mass fraction of constituent i in stream entering melter
 Q_o = total flow rate into off-gas system, kg oxide/hr
 Q_f = total flow rate into 1st melter region, kg oxide/hr
 N = number of constituents.

If no data are available from the off-gas system, decontamination factors are used to calculate the amount of material going to the off-gas system. Under these circumstances, Equations (2.13) and (2.14) are replaced with

$$Q_{io} = Q_e * X_{ie} * (1/DF_i) \quad (2.17)$$

$$Q_{if} = Q_e * X_{ie} * (DF_i - 1)/DF_i \quad (2.18)$$

where DF_i is the melter decontamination factor of constituent i .

It should be recognized that Equations (2.17) and (2.18) do not properly account for losses to the off-gas system during periods of melter idling or low feed rates. For example, according to these equations, there are no losses when the feed rate is zero. Equations (2.13) and (2.14) will model losses at low or zero feed rates, but the losses will be constant over time rather than varying with feed rate; i.e., when the feed rate is zero, losses will be non-zero and will come from the first region in the melter. This part of MASBAL may require refinement at some future date when more is known about off-gas losses as a function of feed rate. However, the errors introduced by Equations (2.13) and (2.14) or (2.17) and (2.18) are small for most constituents because the amount of material going to the off-gas system is generally small relative to the amount going to the glass.

2.5 SIMULATION OF THE SYSTEM

MASBAL treats the operation of the vitrification system as a classical simulation problem. The state of the system at any point in time is defined by the values of the state variables in the system. The state variables include all the masses, concentrations, and flow rates in the system. These variables must be initialized at the start of the simulation, and their values change during the simulation according to the differential and state equations in Section 2.4. The equations are solved simultaneously using a numerical differentiation algorithm.

The differential and state equations alone, however, do not completely describe the behavior of the system. During the operation of the vitrification plant, many events occur that cause instantaneous changes in the state of the system. In simulation jargon, these events are called "discrete events" because they occur at discrete points in time. Examples of discrete events are the starting or stopping of a slurry transfer from the makeup tank to the feed tank, the sampling of the feed tank, and the starting or stopping of a glass pour. Discrete events are triggered either by a condition on time or by a condition on one or more of the state variables. An example of the former is the starting of a batch glass pour every 2 hours. An example of the latter is stopping the flow of feed to the melter when the glass level in the melter exceeds some maximum level. The discrete events that occur when the West Valley CTS is operated are listed in Table 2.1. When these events occur, they alter either the state of the system or the rate of change of the state of the system.

To properly simulate the vitrification system, a model must be capable of simulating both the continuous and the discrete changes in the state of the system. MASBAL makes use of the SIMAN simulation language, a FORTRAN-based software package, to provide these capabilities.

2.5.1 Use of SIMAN

The SIMAN simulation language offers 1) a variable-step, fourth-fifth order Runge-Kutta-Fehlberg numerical differentiation algorithm for solving the mass balance differential equations describing the vitrification system; 2) the

TABLE 2.1. Discrete Events in the West Valley Component Test System

1. Start the flow of slurry from the makeup tank to the feed tank (i.e., the initiation of a batch transfer of feed slurry)
2. Stop the flow of slurry from the makeup tank to the feed tank
3. Change the slurry feed rate to the melter (includes starting or stopping the feed)
4. Start the flow of slurry from the cold chemical makeup tank to the feed tank
5. Stop the flow of slurry from the cold chemical makeup tank to the feed tank
6. Start the flow of slurry from the cold chemical makeup tank to the melter
7. Stop the flow of slurry from the cold chemical makeup tank to the melter
8. Start a glass pour
9. Stop a glass pour

capability to model discrete events that interact with or change the values of state variables in the system; and 3) the capability to introduce stochasm into the simulation. The first capability is essential to the operation of MASBAL because the continuous behavior of the vitrification system is described by a large number of coupled differential equations (see Section 2.4). The second capability is desirable because it simplifies the modeling of discrete behavior in the system (see Table 2.1). The third capability, is essential when MASBAL is run in the second or third modes described in Section 2.3.

SIMAN enables the development of a simulation model that has all these capabilities with a minimum of programming effort. The programmer has only to develop subroutines that describe system-specific behavior. These subroutines are then linked with the main SIMAN subprogram library to create an executable image that draws on the SIMAN software to perform essentially all of the complicated operations associated with simulating the system. The SIMAN software is available from Systems Modeling Corp., State College, Pennsylvania.

2.5.2 MASBAL Implementation

MASBAL consists of FORTRAN subroutines that are integrated with the SIMAN simulation language. During a run, MASBAL reads several input files that contain data that drive the simulation. Once a run is initiated, there are no interfaces between the program and the user other than the error messages that appear if erroneous input is detected (i.e., the program does not have interactive features).

The overall logic in MASBAL is depicted in Figure 2.5. When MASBAL is executed, the simulation clock is initially set to zero and a call is made to the PRIME subroutine. This subroutine calls several subroutines that open input files and read data from these files. These data include 1) parameters specifying various options for running the program, 2) design parameters for the melter system, 3) initial values of state variables in the system, 4) the times at which the initial discrete events occur in the system, and 5) the parameters of statistical distributions that describe uncertainties in process measurements. The names of the subroutines that PRIME calls and brief descriptions of their functions are provided in Table 2.2.

After PRIME has completed execution, control is passed to the differential equation solving algorithm of SIMAN. This algorithm makes frequent calls to the STATE subroutine, which contains the FORTRAN-coded differential and state equations that describe the flow of mass through the vitrification system. SIMAN advances the simulation clock and updates the values of the state variables (as dictated by the equations in STATE) with each time step.

During each time step, SIMAN checks conditions on time and on the state of the system to see if a discrete event is to occur. SIMAN keeps track of the discrete events that are conditional on time by maintaining a special file called the event calendar. This file contains an ordered list of all events that are scheduled to occur in the future and the exact time at which they are to occur. The user specifies all the information needed to schedule these events by setting up the MASBAL input files described in Chapter 3.0. SIMAN also keeps track of events that are conditional on the state of the system. These events occur only when the values of certain state variables cross threshold values that are specified by the user in the MASBAL input files. For

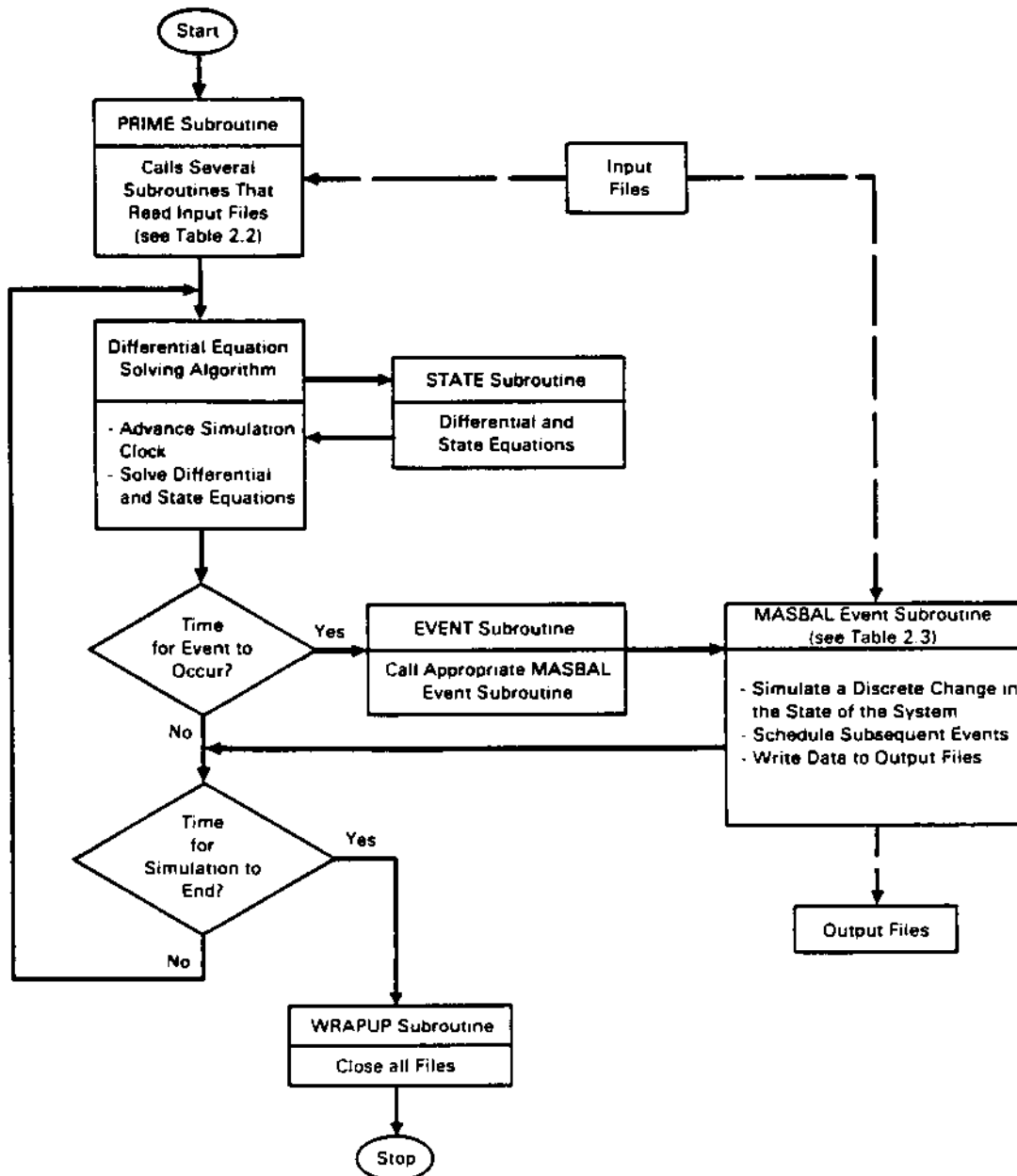


FIGURE 2.5. Flow Diagram of Logic in MASBAL

example, a discrete event that corresponds to shutting off the flow of feed to the melter will occur when the mass of glass in the melter exceeds some maximum value specified by the user (this event will not occur if the feed is scheduled to be shut off at a later time).

If a discrete event is to occur during a time step, the size of the step is adjusted so that it ends when the event is to begin. After the time step is taken, a call is made to the EVENT subroutine. This subroutine passes control to the appropriate MASBAL subroutine that contains logic describing the event

TABLE 2.2. Subroutines Called by PRIME

<u>Name</u>	<u>Description</u>
MODERD	Reads in all the data from the input file MODE.DAT
DSNRD	Reads in all the data from the input file DESIGN.DAT
INITRD	Reads in all the data from the input file INIT.DAT, and initializes all the state variables in the system
FEEDRD	Reads in the first set of data from the input file FEED.DAT, and schedules the first change in the feed rate to the melter (called only in modes 1 and 2)
POURRD	Reads in the first set of data from the input file POUR.DAT, and schedules the first glass pour (called only in modes 1 and 2)
BATRD	Reads in the first set of data from the input file BATCH.DAT, and schedules the first transfer of slurry from the makeup tank to the feed tank (called only in modes 1 and 2)
OFFRD	Reads in the first set of data from the input file OFFGAS.DAT, and schedules the first change in the volatilization rate to the off-gas system (called only in modes 1 and 2)
FSHRD	Reads in the first set of data from the input file FSHIM.DAT, and schedules the first transfer of slurry from the cold chemical makeup tank to the feed tank (called only in modes 1 and 2)
MSHRD	Reads in the first set of data from the input file MSHIM.DAT, and schedules the first transfer of slurry from the cold chemical makeup tank to the melter (called only in modes 1 and 2)
STOCRD	Reads in all the data from the input file STOCH.DAT (called only in modes 2 and 3)

(e.g., a change in the feed rate to the melter, the initiation of a glass pour). In a strict sense, it is not necessary that an event change the state of the system. For example, an event may do nothing more than write the value of a state variable to an output file. The names of the MASBAL event subroutines and brief descriptions of their functions are provided in Table 2.3.

As Table 2.3 indicates, subsequent events are often scheduled from within event subroutines. The times at which the events are scheduled to occur are either read directly from the MASBAL input files, or determined indirectly from

TABLE 2.3. MASBAL Event Subroutines

Name	Description
FUTBAT	Starts the transfer of slurry from the makeup tank to the feed tank on the condition that the level in the feed tank is below some value specified by the user. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file BATCH.DAT has been exhausted. When MASBAL is run in mode 3, FUTBAT is called for all transfers of slurry from the makeup tank to the feed tank. FUTBAT simulates batch-to-batch variability in the feed composition if MASBAL is run in modes 2 or 3.
FUBSTP	Stops the transfer of slurry from the makeup tank to the feed tank on the condition that the level in the feed tank is above some value specified by the user. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file BATCH.DAT has been exhausted. When MASBAL is run in mode 3, FUBSTP is called for all transfers of slurry from the makeup tank to the feed tank.
STOPFD	Stops the flow of feed to the melter on the condition that the level of glass in the melter is above some value specified by the user. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file FEED.DAT has been exhausted. When MASBAL is run in mode 3, STOPFD is called whenever the melter level condition is met.
STRTFD	Starts the flow of feed to the melter (after a stoppage) on the condition that the level of glass in the melter is below some value specified by the user. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file FEED.DAT has been exhausted. When MASBAL is run in mode 3, STRTFD is called whenever the melter level condition is met.
STOPPR	Stops a glass pour on the condition that the level of glass in the melter is below some value specified by the user. Writes the mass and composition of the pour to the appropriate output files. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file POUR.DAT has been exhausted. When MASBAL is run in mode 3, STOPPR is called whenever the melter level condition is met.

TABLE 2.3. (contd)

Name	Description
STRTPR	Starts a glass pour (after a stoppage) on the condition that the level of glass in the melter is above some value specified by the user. When MASBAL is run in modes 1 or 2, this subroutine is called only after all the data in the input file POUR.DAT has been exhausted. When MASBAL is run in mode 3, STRTPR is called whenever the melter level condition is met.
FUTPOR	Starts a glass pour that is scheduled to occur after all the data in the input file POUR.DAT has been exhausted. Schedules the subsequent stoppage of the pour.
FUPSTP	Stops a glass pour that is scheduled to occur after all the data in the input file POUR.DAT has been exhausted. Writes the mass and composition of the pour to the appropriate output files. Schedules the next pour.
BSTART	Starts a scheduled transfer of slurry from the makeup tank to the feed tank. Schedules the subsequent stoppage of the transfer. Reads either the measured composition in the feed tank (after the transfer) from the input file BATCH.DAT, or the apparent composition in the makeup tank (before the transfer) from the input file MAKEUP.DAT. Simulates sampling and analytical error if MASBAL is run in modes 2 or 3.
BSTOP	Stops a scheduled transfer of slurry from the makeup tank to the feed tank. Reads an additional line from the input file BATCH.DAT, and schedules a subsequent transfer.
CHFEED	Changes the flow rate of feed to the melter based on information in the input file FEED.DAT. Reads an additional line from FEED.DAT, and schedules the next change in the feed rate.
PSTART	Starts a scheduled glass pour. Schedules the subsequent stoppage of the pour.
PSTOP	Stops a scheduled glass pour. Writes the mass and composition of the pour to the appropriate output files. Reads another line from the input file POUR.DAT, and schedules the next pour.

TABLE 2.3. (contd)

Name	Description
FSHIM	Starts a scheduled transfer of slurry from the cold chemical makeup tank to the feed tank. Schedules the subsequent stoppage of the transfer. Reads the apparent composition in the cold chemical makeup tank from the input file FSHIM.DAT. Simulates sampling and analytical error or slurry preparation error if MASBAL is run in modes 2 or 3.
FSTOP	Stops a scheduled transfer of slurry from the cold chemical makeup tank to the feed tank. Reads an additional line of the input file FSHIM.DAT, and schedules the next transfer.
MSHIM	Starts a scheduled transfer of slurry from the cold chemical makeup tank to the melter. Schedules the subsequent stoppage of the transfer. Reads the apparent composition in the cold chemical makeup tank from the input file MSHIM.DAT. Simulates sampling and analytical error or slurry preparation error if MASBAL is run in modes 2 or 3.
MSTOP	Stops a scheduled transfer of slurry from the cold chemical makeup tank to the melter. Reads an additional line of the input file MSHIM.DAT, and schedules the next transfer.
OFFGAS	Changes the rate of volatilization (of each constituent) to the offgas system based on information in the input file OFFGAS.DAT. Simulates off-gas sampling and analytical errors if MASBAL is run in modes 2 or 3. Reads an additional line of OFFGAS.DAT, and schedules the next change in the volatilization rate.
RECORD	Writes the composition (mass fraction of each constituent) in the last region of the melter to the appropriate output files. This subroutine is called at regular intervals specified by the user.

the design parameters specified by the user. The scheduling of discrete events is a function that is performed internally within MASBAL by making calls to appropriate SIMAN subroutines. The interested reader is referred to Pegden (1985) for a complete discussion of how discrete events are scheduled using SIMAN subroutines.

After a MASBAL event subroutine has completed execution, control is passed back to the differential equation-solving algorithm of SIMAN. The simulation resumes with calls to the STATE or EVENT subroutines as necessary. Each time the simulation clock is advanced, SIMAN checks to see if the new time is greater than or equal to the time specified for ending the simulation. If it is greater, the time step is adjusted so that it ends at the specified time. When the ending time is reached, the simulation is stopped and a call is made to the WRAPUP subroutine, which closes all input and output files. After the files are closed, a FORTRAN STOP is executed.

A listing of the MASBAL source code (excluding the proprietary SIMAN software) is provided on microfiche in a pocket on the inside of the front cover of this report. For those who are interested, a hardcopy listing can be obtained directly from the author.

2.5.3 State Variables

MASBAL contains over 1900 state variables that define the state of the simulated system at any point in time. The state variables correspond to the values of

- total volumes or masses in tanks or melter regions
- masses of individual constituents in tanks or melter regions
- concentrations or mass fractions of constituents in tanks, melter regions, and streams
- flow rates.

All of the state variables are contained in the array S(I), which has 2000 locations. Figure 2.6 and Table 2.4 show the correspondence between the state variables and the physical variables in the vitrification system. It should be noted that not all of the state variables are used in every run of

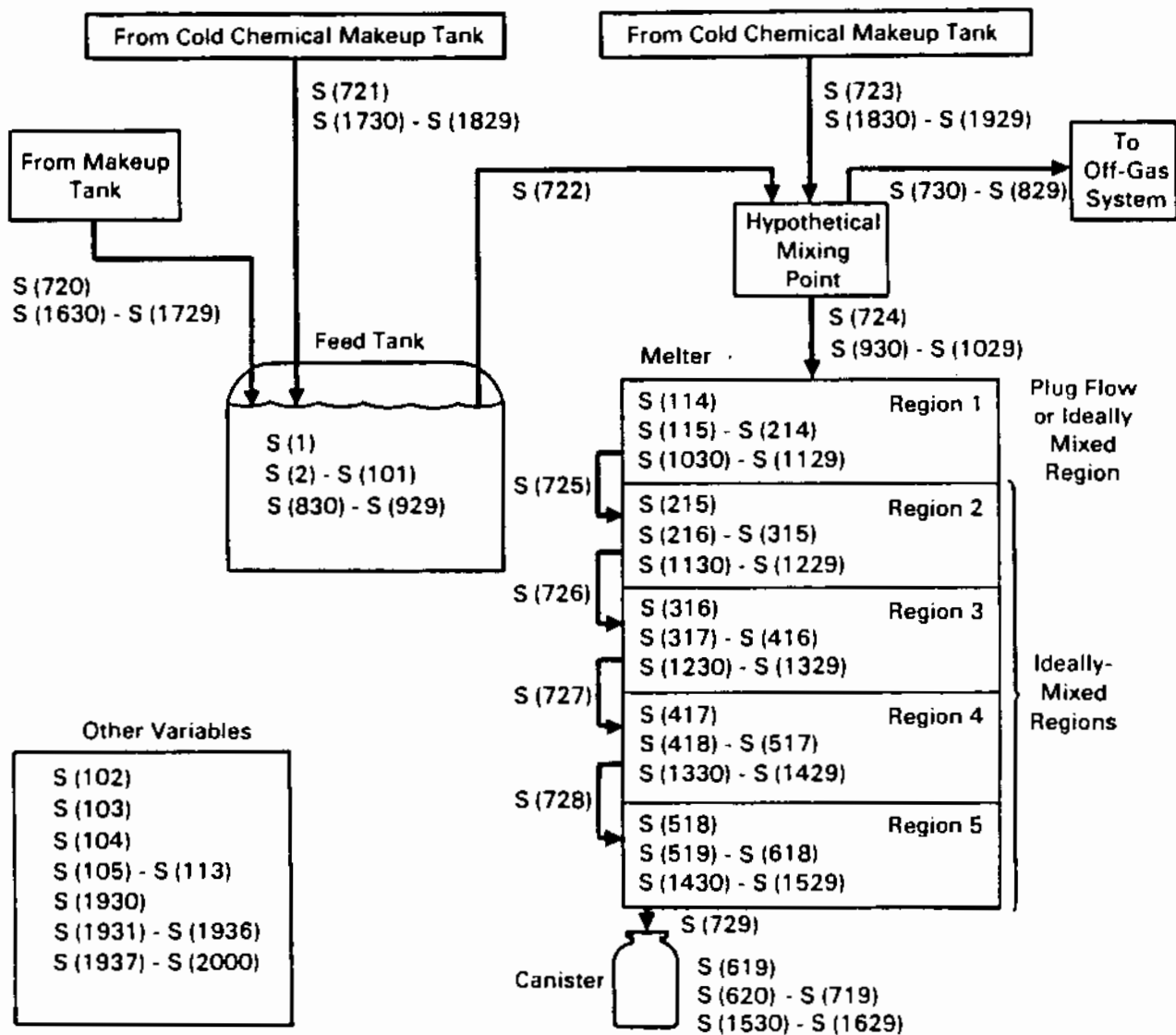


FIGURE 2.6. Correspondence Between State Variables and Physical Variables in MASBAL (NOTE: See Table 2.4 for Key)

MASBAL. If less than 100 constituents are specified, for example, many of the array locations corresponding to the masses and concentrations of constituents in the feed tank and the various regions in the melter will not be used. Also, if the melter is modeled as having less than five regions, only the variables for the specified number of regions will be used in the mass balance calculations. Any regions that are not used are bypassed in the mass balance calculations.

TABLE 2.4. Key to Figure 2.6

S(1)	Total Volume in Feed Tank (L)
S(2)-S(101)	Masses of Individual Constituents in Feed Tank (g oxide)
S(102)	Cumulative Mass into Region 1 in Melter (g oxide)
S(103)	Cumulative Mass out of Region 1 in Melter (g oxide)
S(104)	Total Mass of Glass in Melter (g oxide)
S(105)-S(113)	Currently not used
S(114)	Total Mass of Region 1 in Melter (g oxide)
S(115)-S(214)	Masses of Individual Constituents in Region 1 (g oxide)
S(215)	Total Mass of Region 2 in Melter (g oxide)
S(216)-S(315)	Masses of Individual Constituents in Region 2 (g oxide)
S(316)	Total Mass of Region 2 in Melter (g oxide)
S(317)-S(416)	Masses of Individual Constituents in Region 3 (g oxide)
S(417)	Total Mass of Region 4 in Melter (g oxide)
S(418)-S(517)	Masses of Individual Constituents in Region 4 (g oxide)
S(518)	Total Mass of Region 5 in Melter (g oxide)
S(519)-S(618)	Masses of Individual Constituents in Region 5 (g oxide)
S(619)	Total Mass of Current Glass Pour (g oxide)
S(620)-S(719)	Masses of Individual Constituents in Glass Pour (g oxide)
S(720)	Flow Rate from makeup Tank (L/hr)
S(721)	Flow Rate from Cold Chemical Makeup Tank to Feed Tank (L/hr)
S(722)	Flow Rate from Feed Tank to Melter (L/hr)
S(723)	Flow Rate from Cold Chemical Makeup Tank to Melter (L/hr)
S(724)	Net Mass Flow Rate into Melter (g oxide/hr)
S(725)	Mass Flow Rate from Region 1 to Region 2 (g/hr)
S(726)	Mass Flow Rate from Region 2 to Region 3 (g/hr)
S(727)	Mass Flow Rate from Region 3 to Region 4 (g/hr)
S(728)	Mass Flow Rate from Region 4 to Region 5 (g/hr)
S(729)	Mass Flow Rate from Region 5 in Melter to Canister (g/hr)
S(730)-S(829)	Mass Flow Rates of Individual Constituents to Off-Gas System (g oxide/hr)
S(830)-S(929)	Concentrations of Individual Constituents in Feed Tank (g oxide/L)
S(930)-S(1029)	Mass Fractions of Individual Constituents in Flow into Melter
S(1030)-S(1129)	Mass Fractions of Individual Constituents in Region 1
S(1130)-S(1229)	Mass Fractions of Individual Constituents in Region 2
S(1230)-S(1329)	Mass Fractions of Individual Constituents in Region 3
S(1330)-S(1429)	Mass Fractions of Individual Constituents in Region 4
S(1430)-S(1529)	Mass Fractions of Individual Constituents in Region 5
S(1530)-S(1629)	Mass Fractions of Individual Constituents in Glass Pour
S(1630)-S(1729)	Concentrations of Individual Constituents in Makeup Tank (g oxide/L)
S(1730)-S(1829)	Concentrations of Individual Constituents in Cold Chemical Makeup Tank (g oxide/L)
S(1830)-S(1929)	Concentrations of Individual Constituents in Cold Chemical Makeup Tank (g oxide/L)
S(1930)	Total Mass Flow Rate into Melter (g oxide/hr)
S(1931)-S(1938)	Input Values That Are Used to Trigger Discrete Events
S(1937)-S(2000)	Currently Not Used

The values of the state variables can change during the simulation in two ways: 1) as prescribed by the differential and state equations in the STATE subroutine, and 2) as dictated by statements in MASBAL event subroutines. The first type of change is a continuous change, such as the gradual increase in mass fraction of a constituent in the melter after an increase in the concentration of the constituent in the feed. The second type of change is a discrete change, such as the stopping of a glass pour.

2.5.4 Stochasm in MASBAL

When MASBAL is run in either the second or the third mode (see Section 2.3), it simulates random errors in process measurements and inherent fluctuations in the feed composition (mode 3 only). MASBAL does this by randomly sampling statistical distributions that represent these errors or fluctuations. The most likely values of these distributions are either the actual values of process measurements (when simulating measurement errors) or the target or design concentrations of constituents in the feed (when simulating inherent fluctuations in the feed composition). The parameters that define the shapes of the distributions (e.g., standard deviations, minima, maxima) are specified by the user.

Random sampling of the statistical distributions is accomplished by calls to appropriate SIMAN subroutines. Whenever a distribution is to be sampled, the parameters that define the distribution (e.g., the mean and standard deviation for a normal distribution) are passed to SIMAN as arguments in a subroutine call list. Control is then passed to a SIMAN algorithm that generates random numbers. After a random number is generated, a special SIMAN function translates the number to a representative value from the specified statistical distribution. This value is then returned to MASBAL as either the value of a process measurement or the concentration of a constituent in the feed.

2.6 MASBAL FILES

The complete MASBAL software package consists of the following files:

- 35 FORTRAN source (text) files

- 11 text files containing MASBAL common blocks
- 35 FORTRAN object files (compiled source files)
- 2 special text files: the SIMAN experiment file (MASBAL.EXP) and the SIMAN model file (MASBAL.MOD)
- 2 special object files (MASBAL.E and MASBAL.M) created by "processing" the experiment file and the model file with SIMAN processing programs
- 1 special program file created by the SIMAN linker program (MASBAL.P)
- 2 executable images of MASBAL created by linking the 35 FORTRAN object files with 4 SIMAN object files - One image is the production version of MASBAL, and the other is the debug version
- 11 input files
- several output files (the number varies depending on which version and which mode of MASBAL is run)
- 6 VAX/VMS command files that facilitate the compiling, linking, and execution of MASBAL.

The special SIMAN files and the two versions of MASBAL are discussed in greater detail in this section. The input files are the topic of Chapter 3.0, and the output files are discussed in Chapter 4.0.

2.6.1 Special SIMAN Files

In addition to all the FORTRAN files that comprise MASBAL and SIMAN, two special text files are included as part of the MASBAL software package. These files are the SIMAN model file and the SIMAN experiment file. The model file (MASBAL.MOD) is an empty file that exists only because it is required for execution of SIMAN. The experiment file (MASBAL.EXP) contains some important parameters that specify 1) dimensions of internal SIMAN arrays; 2) the minimum and maximum time step sizes and the maximum absolute and relative truncation errors for each time step taken by the Runge-Kutta-Fehlberg differential equation solving algorithm; and 3) conditions that trigger discrete events that are conditional on the state of the system. A listing of the MASBAL experiment

file is included at the end of Appendix A. The reader is referred to Pegden (1985) for a complete explanation of each of the elements in this file. The casual MASBAL user need not be concerned with this file, as all the parameters have been adjusted for proper MASBAL execution.

Before MASBAL can be run, both the model file and the experiment file must be "processed" by SIMAN. The model file is processed by running a program called the SIMAN model processor, and the experiment file is processed by running the SIMAN experiment processor. These processors interpret the information in the respective text files and create object files called MASBAL.M and MASBAL.E. The two object files are then linked to create a file called MASBAL.P. This is accomplished by running a program called the SIMAN linker. MASBAL.P must reside in the same work area as the MASBAL executable image or MASBAL will not run. The casual user need not be concerned with processing and linking the model and experiment files, as the MASBAL.P file has already been created and is provided in the MASBAL software package.

2.6.2 Versions of MASBAL

Two versions of MASBAL are available to the user: a production version and a debug version. The only difference between the two versions is that the debug version generates more output files. The additional files are useful for determining the exact sequence of events that occurred during the simulation and for debugging the program. The production version runs somewhat faster than the debug version, because it does not access the disk as frequently. The debug version should be used when setting up new problems, as it is much easier to find errors in the input files when this version is run. The production version should be used when relatively minor changes are made to the inputs from one run to the next, or when a simulation is repeated several times to obtain a distribution of results (i.e., modes 2 or 3). The output generated by the two versions is discussed in Chapter 4.0.

The FORTRAN coding for the two versions of MASBAL is identical except for the value of the variable NDEBUG in the PRIME subroutine. NDEBUG is used as a flag that tells MASBAL which set of output files to generate. In the production version, NDEBUG is set equal to zero, while in the debug version it is set

equal to 1. NDEBUG can be changed only by editing the source file PRIME.FOR; it cannot be changed from outside the program (i.e., via an input file). Both versions of MASBAL are included in the MASBAL software package.

3.0 INPUT FILES

The MASBAL input files represent the only interface between MASBAL and the user. Before each run of MASBAL, the input files must be modified to reflect the changes that the user wants to make since the previous run. The modifications should be made using a text editor such as the EDT editor (on DEC VAX computers running the VMS operating system). The program is then executed, and all input data are processed in the proper order.

MASBAL has a total of 11 input files. These files and the modes of operation in which they are used are listed in Table 3.1.

TABLE 3.1. MASBAL Input Files and Modes of Operation in Which They Are Used

<u>File</u>	<u>Mode(s)</u>
MODE.DAT	1,2,3
DESIGN.DAT	1,2,3
INIT.DAT	1,2,3
FEED.DAT	1,2
POUR.DAT	1,2
BATCH.DAT	1,2
MAKEUP.DAT	1,2
OFFGAS.DAT	1,2
FSHIM.DAT	1,2
MSHIM.DAT	1,2
STOCH.DAT	2,3

In the deterministic mode (mode 1), all files except STOCH.DAT are used. In mode 2, all files are used. In mode 3, only MOOE.DAT, DESIGN.DAT, INIT.DAT, and STOCH.DAT are used.

All of the input files are set up so that the user can quickly see where each input value is to be entered. The files are partially self-documenting, as they contain blocks of text that describe the inputs. All input values are

read from formatted fields. The formatting is indicated by asterisks and decimal points directly above the field from which the value is read. The following example serves to illustrate this.

Suppose a file contains these two lines:

```
INITIAL FEED RATE (L/HR) = ***.***
```

In this case, the user will know 1) the value is to be entered in units of liters/hr, 2) the format field is F7.3 (for a real number with three places before and three places after the decimal point), and 3) the field starts in the second space after the equal sign. The user might enter the input value as follows:

```
***.***  
INITIAL FEED RATE (L/HR) = 120.0
```

It is very important that the inputs in each file be properly formatted, or MASBAL will not run correctly.

Each input file and its contents are discussed in detail in this chapter. Examples of each file are provided in Appendix A (these are copies of printouts of input files that have been used in MASBAL runs).

3.1 MODE.DAT

This file contains input data that control the logic in the simulation. The inputs are:

- MODE - The user must choose 1, 2, or 3. The three modes are discussed in detail in Section 2.3. If the user chooses any number other than 1, 2, or 3, the code will give an error message.
- LENGTH OF SIMULATION - The amount of real time that MASBAL simulates in a given run. The value must be specified in hours.
- NUMBER OF REPEAT SIMULATIONS - The number of repeat runs that MASBAL performs when the code is run in modes 2 or 3. The runs will be

identical except that each one will use a different random number stream for sampling statistical distributions. Each run, therefore, will give a slightly different set of results. The distribution of results over many runs can be used to establish confidence limits about the results obtained when the code is run in mode 1. When MODE = 1, the number of repeat simulations defaults to 1.

- TIME INTERVAL FOR RECORDING COMPOSITION IN MELTER - This input is used to specify the time interval (in hours) for writing the predicted composition in the melter to the output files COMP1.OUT through COMPx.OUT (see Chapter 4.0). The default value is 5 hours.
- COMPOSITION OF FUTURE BATCHES OF FEED - The user must choose 1 or 2 (1 for target, 2 for same composition as last batch of feed). This input is used in modes 1 or 2 when the process data provided in the files BATCH.DAT and MAKEUP.DAT runs out before the simulation completes. For example, if the user provides data for only two batches of feed, but the simulation requires four batches in order to run the specified length of time, MASBAL will automatically set the composition of the last two batches of feed equal to either the target composition or the same composition as the last batch of feed. When the code is run in mode 3, this input defaults to 1 (target).
- NUMBER OF BATCHES - This input is used only if 2 is chosen as the input for the COMPOSITION OF FUTURE BATCHES OF FEED; it is ignored otherwise. The value specifies the number of consecutive batches of feed that should have the same composition as the last batch. After this number of batches has been processed, all further batches will have the target composition.
- NUMBER OF SAMPLES OF FEED PER BATCH - This input is used only if MODE = 2 or 3, and only for "future" batches if MODE = 2. The value must be an integer between 1 and 5. This value represents the number of replicate samples that are to be taken of the feed prior to transfer from the makeup tank to the feed tank.

- NUMBER OF ANALYSES PER SAMPLE OF FEED - This input is used only if MODE = 2 or 3, and only for "future" batches if MODE = 2. The value must be an integer between 1 and 3. This value represents the number of replicate analyses that are performed on each sample of feed taken from the makeup tank prior to transfer to the feed tank.
- OPTION - This is the option for modeling the mixing behavior in the melter. The user must choose 1, 2, or 3. If 1 is chosen, the melter will be modeled as a single ideally-mixed tank. If 2 is chosen, the melter will be modeled as a plug flow region followed by one or two ideally-mixed regions in series. If 3 is chosen, the melter will be modeled as two to five ideally-mixed regions in series. If the user chooses any number other than 1, 2, or 3, the code will give an error message.
- NUMBER - This input reflects the number of ideally-mixed regions that are to be modeled in the melter. If OPTION = 1, the input is ignored because this option pertains to only one ideally-mixed tank. If OPTION = 2, the user must specify 1 or 2. If OPTION = 3, the user must specify 2 to 5. Any numbers other than those mentioned here will give error messages.
- VOLUME PERCENTAGES OF REGIONS IN MELTER - This input is the steady-state volume percentages of each region in the melter (i.e., when the melter is operating at the design feed rate and the design feed oxide loading). The entries must be consistent with the option and the number of ideally-mixed regions specified in the preceding two inputs. For example, if OPTION = 2 and NUMBER = 2 (one plug flow and two ideally-mixed regions), then a non-zero value should be specified under each of the first three locations. If OPTION = 2, the first region is always considered to be the plug flow region. Ideally-mixed regions should always be ordered from smallest to largest volume percentage. The volume percentages must add up to 100.0 exactly or an error message will result. When OPTION = 1, the input is ignored.

3.2 DESIGN.DAT

This file contains all the design parameters for the vitrification system. The parameters can be modified to accommodate any change in the design of the system. The inputs are:

- CONSTITUENTS, TARGET COMPOSITION, and DECONTAMINATION FACTOR - These inputs are entered in tabular form under the appropriate column headings near the top of the file ("Constituent", "Mass Frac.", and "Decon. Factor"). Each constituent must be specified as an alphanumeric character string not more than 8 characters in length. The alphanumeric string should always start under the first asterisk that specifies the "Constituent" format field. All constituents that are to be included in the model must appear in the constituent list in this file. The target glass composition (mass fraction) and the melter decontamination factor for each constituent should be entered to the right of the constituent name. The list of constituent names should always end with the string END. As MASBAL reads the input file, it looks for the string END to tell it when to stop reading constituent names. If END is not there, the run will terminate with error status.
- TARGET OXIDE LOADING OF FEED - the target oxide loading of the feed slurry in grams per liter
- TARGET DENSITY OF FEED SLURRY - the target density of the feed slurry in grams per cubic centimeter
- TARGET DENSITY OF GLASS - The target density of the glass in grams per cubic centimeter
- VOLUME CORRECTION FOR STEAM JET - This input specifies a volume correction factor for the amount of water that is added to the feed during transfer from the makeup tank to the feed tank by steam jet. The units are liters of feed per liter of makeup tank slurry. The volume correction factor should always be greater than one.
- TRANSFER RATE FROM MAKEUP TANK TO FEED TANK - the transfer rate in liters per hour

- RATE OF ADDITION OF "SHIMS" - the rate of addition of glass formers to either the feed tank or the melter in liters per hour
- FEED RATE TO MELTER - the design feed rate to the melter in liters per hour
- GLASS POURING RATE - the design pouring rate of glass from the melter in kilograms per hour
- DURATION OF EACH GLASS POUR - the duration of each glass pour in hours
- TIME BETWEEN POURS - the duration between glass pours in hours
- VOLUME IN FEED TANK AFTER FILLING - the volume of slurry, liters, in the feed tank after each transfer from the makeup tank; this volume does not necessarily have to be the capacity of the feed tank.
- VOLUME OF HEEL IN FEED TANK - the volume of slurry, liters, in the feed tank prior to each transfer from the makeup tank (in liters)
- DESIGN WORKING VOLUME OF MELTER - the volume of glass, liters, that the melter is designed to hold
- MAXIMUM VOLUME OF GLASS ALLOWED IN MELTER - the maximum volume of glass, liters, that the melter will safely accommodate
- MINIMUM VOLUME OF GLASS ALLOWED IN MELTER - the minimum volume of glass, liters, that the melter will safely accommodate.
- PARAMETER FOR ADJUSTMENT OF TIME CONSTANT - the value of the parameter β in Equations (2.7) and (2.8) of this report. This parameter is used to adjust the time that it takes for the mass of regions in the melter to respond to changes in the feed rate. A value from 1 to 5 is recommended.

3.3 INIT.DAT

This file is used to specify initial values for the simulation. The initial values are assumed to be based on process measurements that are taken prior to the start of a run. The inputs are:

- INITIAL COMPOSITION IN FEED TANK - The inputs are entered in tabular form under the first set of column headings in the file. Alpha-numeric constituent names are entered in the "Constituent" column. These constituent names must be identical to the names used in the constituent list in DESIGN.DAT. If a constituent name does not match up with any constituent in DESIGN.DAT, an error message will result (a typographical error could cause this to happen). If a constituent is omitted from the list, MASBAL will assume that the initial composition of that constituent in the feed tank is zero. A constituent name may appear more than once in the "Constituent" column. Replicate constituent names indicate that replicate samples were taken of the feed. To the right of each constituent name, the user must enter the results of one to three analyses (for that constituent) in units of grams oxide/liter. The user should enter the number of analyses in the column labeled "No. Anal." (this must be an integer from 1 to 3). An example best illustrates this. Suppose the following lines are entered in the table:

CONSTITUENT	ANAL.	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
*****	*	***.***	***.***	***.***
SI02	3	157.5	162.5	162.5
SI02	2	152.5	154.5	151.5

MASBAL will interpret these lines as follows: Two samples were taken from the feed tank. The first sample was analyzed three times for SI02, with the results of the analyses being 157.5, 162.5, and 162.5 g oxide/liter, respectively. The second sample was analyzed twice for SI02, with the results of the analyses being 152.5 and 154.5 (the 151.5 is ignored in this case). The value taken as the initial composition in the feed tank will be the average of the five analyses. As with the constituent list in DESIGN.DAT, the constituent list here must end with the string END or else the run will terminate with errors.

- INITIAL COMPOSITION IN MELTER - The inputs are entered in the same manner as for INITIAL COMPOSITION IN THE FEED TANK except that the values are in units of mass fraction.
- INITIAL VOLUME IN FEED TANK - the initial volume of slurry, liters, in the feed tank
- INITIAL VOLUME OF GLASS IN MELTER - the initial volume of glass, liters, in the melter
- INITIAL FEED RATE TO MELTER - the initial feed rate to the melter, in liters per hour
- INITIAL VOLUME PERCENTAGES OF REGIONS IN MELTER - The volume percentages of each region in the melter at the start of the simulation. The entries must be consistent with the OPTION and the NUMBER of ideally-mixed regions specified in MODE.DAT. The order of the regions must be the same as in MODE.DAT. The last ideally-mixed region is the only region that must be specified as having an initial volume greater than zero. If the melter is idling prior to the start of a run, it is probably in a relatively ideally-mixed state. This situation can be simulated by specifying that all regions in the melter except the last region have an initial volume percentage of zero. All initial volume percentages must add up to 100.0 exactly or an error message will result. When OPTION = 1, the input is ignored.

3.4 FEED.DAT

This file contains input data specifying the times of changes in the feed rate and the new feed rate when these changes occur. The inputs must be ordered sequentially. Times (in hours) are entered in the "Time" column and rates (in liters per hour) are entered in the "Rate" column. The last line in the file should always be the last line of data; if the file ends with a blank line, the code will give unpredictable results. If there are no data, then the last line should be the line containing the asterisks that specify the format fields. In this case, the feed rate for the entire simulation will be equal to the initial feed rate specified in INIT.DAT.

3.5 POUR.DAT

This file contains input data specifying the starting times, stopping times, and masses of each glass pour. The inputs must be ordered sequentially. Starting times (in hours) are entered in the "Start Time" column, stopping times (in hours) are entered in the "Stop Time" column, and masses (in kilograms) are entered in the "Mass of Pour" column. As in the case of FEED.DAT, the last line of data should always be the last line in the file; if this file ends with a blank line, the code will give unpredictable results. If there are no data, then the last line should be the line containing the asterisks that specify the format fields. If no data are specified, MASBAL will simulate glass pours that start and stop at regular intervals as specified by the values for the DURATION OF EACH GLASS POUR and TIME BETWEEN POURS in DESIGN.DAT. The pouring rate will default to the value specified for GLASS POURING RATE in DESIGN.DAT.

3.6 BATCH.DAT

This file contains input data specifying the starting and stopping times of batches to the feed tank and the volume in the feed tank at the beginning and end of each batch. It also contains data specifying the composition in the feed tank after each batch. With the exception of the first six lines in the file (which serve as a header), the entire file should appear as a series of repeated "blocks" of text that are identical except for the numerical values within each block. Each block should start with the line that contains the column headers "Start Time," "Stop Time," "Start Vol," "Stop Vol" and end with the line that has the string END in the "Constituent" column. The blocks should contain data for successive batches of feed (a new block should be added for each batch that is transferred from the makeup tank to the feed tank). The starting and stopping times should be specified in hours and the starting and stopping volumes in the feed tank should be specified in liters. The constituent names and the results of analyses of the samples should be entered exactly as they are in INIT.DAT (see INITIAL COMPOSITION IN FEED TANK in Chapter 3.3). Composition data should be provided for each batch of feed. The data may not be available for the last batch, however, because of the lag time in getting

results back from the analytical laboratory (there may be as much as a 24 hour turnaround time for results from the analytical lab). If this is the case, the last line of the file should be the line containing the starting and stopping times of the last batch of feed (or any line between this line and the line that contains the asterisks used to specify format fields for the analytical results). If composition data are available for the last batch, the last line in the file should be the line that has the string END in the "Constituent" column.

3.7 MAKEUP.DAT

This file is used only if composition data for the last batch of feed to the feed tank are not yet available from the analytical laboratory. MAKEUP.DAT should contain data specifying the composition of the slurry in the makeup tank prior to the last transfer to the feed tank. MASBAL will use the composition in the makeup tank as the composition of the most recent batch (adjusted to account for water added by the steam jet during transfer to the feed tank) until the results from the analytical laboratory are available. The constituent names and the results of analyses of the samples should be entered exactly as they are in INIT.DAT (see INITIAL COMPOSITION IN FEED TANK in Chapter 3.3). This file should be updated every time another batch is transferred from the makeup tank to the feed tank. The last line in this file should always be the line that has the string END in the "Constituent" column.

3.8 OFFGAS.DAT

This file contains input data specifying the times at which samples are taken from the off-gas system and the analytical results from these samples. With the exception of the first five lines in the file (which serve as a header), the entire file should appear as a series of repeated "blocks" of text that are identical except for the numerical values within each block. Each block should start with the line that contains the asterisks specifying the format field for the time at which the sample(s) were taken and end with the line that has the string END in the "Constituent" column. The blocks should contain data for successive sets of samples from the off-gas system (a new

block should be added for each sample or set of samples taken). The sampling times should be specified in hours. The constituent names and the results of analyses of the samples should be entered exactly as they are in INIT.DAT (see INITIAL COMPOSITION IN FEED TANK in Chapter 3.3), except that the values should be in units of grams instead of gram oxide/liter. The last line in this file should always be the line that has the string END in the "Constituent" column.

3.9 FSHIM.DAT

This file contains input data specifying the times at which glass formers are added to the feed tank and the volume and composition of each of these additions. With the exception of the first two lines in the file (which serve as a header), this file should consist of a series of "blocks" of text that are identical except for the numerical values within each block. Each block should contain data for a different addition of glass formers (sequentially ordered). All blocks should start with the line that contains the column headers "Time (hrs)" and "Volume (L)" and end with the line that has the string END in the constituent column. Times should be specified in hours and volumes in liters. For each addition, the user must specify a METHOD OF DETERMINATION of the slurry composition. This number should be specified as either 0 or 1 (the default is 1). The user should specify 1 if the composition of the added slurry is determined by taking samples of the slurry and analyzing these samples, and the user should specify 0 if the composition is known only to the extent that the user knows how the slurry was prepared (i.e., from knowing the amount of each glass former that was added to the slurry). Composition data should be specified in exactly the same way as it is in INIT.DAT (see INITIAL COMPOSITION IN FEED TANK in Chapter 3.3). If METHOD OF DETERMINATION = 1, replicate constituent names may be used to indicate replicate samples, and the results of up to three analyses per sample can be specified in the "Analysis 1," "Analysis 2," and "Analysis 3" columns. If METHOD OF DETERMINATION = 0, however, the user should not enter replicates in the constituent list. Also, when METHOD OF DETERMINATION = 0, only the number in the "Analysis 1" column will be read by MASBAL. The last line in this file should be the line containing the string END in the constituent column. If there are no data, the last line should be the line containing the asterisks that specify the format fields

for "Time" and "Volume." If zero is specified as both the time and volume of the first addition, all other inputs will be ignored and MASBAL will assume that there are no glass former additions to the feed tank.

3.10 MSHIM.DAT

This file contains data specifying the times at which glass formers are added to the melter and the volume and composition of each of these additions. The file is structured exactly like FSHIM.DAT, so the reader is referred to Section 3.9 for a discussion of the inputs.

3.11 STOCH.DAT

This file contains data specifying the statistical distributions that are used to simulate errors in process measurements and inherent fluctuations in process variables. It also contains data specifying the parameters that define these distributions. The distributions and their parameters should be selected on the basis of information obtained from experiments aimed at characterizing the uncertainties in the process. STOCH.DAT is used only when MASBAL is run in modes 2 or 3.

3.11.1 Statistical Distributions

MASBAL offers the user a choice of 10 statistical distributions for simulating errors in process measurements and inherent fluctuations in the feed composition. These distributions are described in detail in this section.^(a) The numbers assigned to the distributions correspond to the numbers that the user must specify in STOCH.DAT when selecting a distribution. The first four distributions always have symmetrical probability density functions. The last six distributions can have either symmetrical or nonsymmetrical distribution functions depending on the parameters that the user specifies. The distributions are:

(a) Additional information about the statistical distribution can be obtained from standard statistics texts such as Choi (1978) and Tsokos (1972).

1. constant (point distribution) - This "distribution" is simply the deterministic value of a variable. It gives the user the option of treating some variables deterministically while treating others stochastically.
2. normal (Gaussian) - The probability density function for this distribution is

$$f(x) = (1/\sqrt{2\pi}\sigma) * \exp\{-0.5 * [(x - \mu)/\sigma]^2\} \quad (3.1)$$

where $-\infty < x < \infty$

μ = mean

σ = standard deviation

The mean of the distribution is the value of the variable that is passed from MASBAL (i.e., the deterministic value).

3. uniform (symmetrical) - This distribution has a rectangular shaped probability density function, as shown in Figure 3.1. The distance between the maximum value of the distribution and the value of the variable that is passed from MASBAL is the same as the distance between the minimum value of the distribution and the value of the variable that is passed from MASBAL.
4. triangular (symmetrical) - This distribution has a triangular shaped probability density function, as shown in Figure 3.2. The distance between the maximum value of the distribution and the value of the variable that is passed from MASBAL is the same as the distance between the minimum value of the distribution and the value of the variable that is passed from MASBAL. The minimum and maximum values both have a probability of zero (thus defining the base of the triangle) and the value of the variable that is passed from MASBAL has the highest probability (thus forming the apex of the triangle).
5. lognormal - The probability density function for this distribution is

$$f(x) = (1/x\sqrt{2\pi\sigma}) * \exp\{-0.5 * [(\ln(x) - \mu)/\sigma]^2\} \quad (3.2)$$

where $x > 0$

μ = mean of $y = \ln(x)$

σ = standard deviation of $y = \ln(x)$

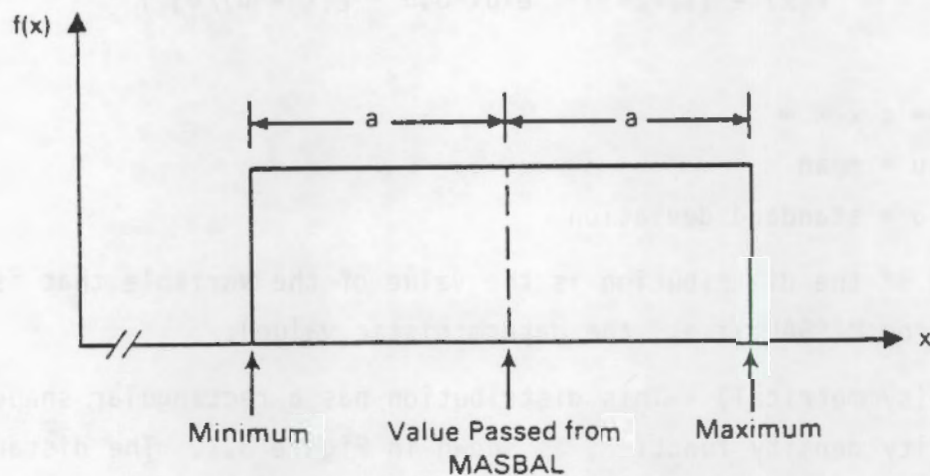


FIGURE 3.1. Probability Density Function for Symmetrical Uniform Distribution

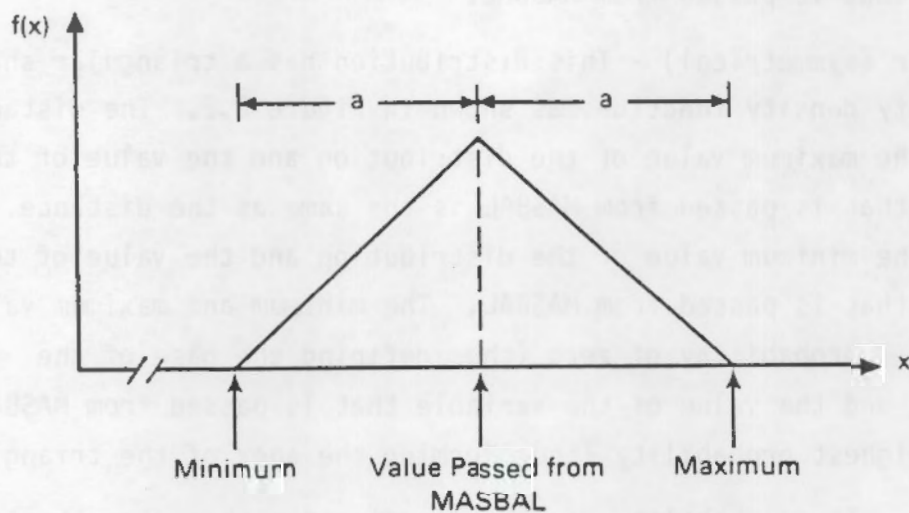


FIGURE 3.2. Probability Density Function for Symmetrical Triangular Distribution

The mode (most likely value) of the distribution is the value of the variable that is passed from MASBAL. Since the lognormal distribution normally has zero as its lower bound, the user must specify an "offset" (as a percentage of the mode). This offset is subtracted from the mode, and the x-axis is transformed so that the offset point is treated as zero. The scale on the transformed axis is adjusted so that the distance between the offset point and the mode is equivalent to $\exp(\mu - \sigma^2)$, which is the distance between zero and the mode when Equation (3.2) is used as the probability density function.

6. gamma - The probability density function for this distribution is

$$f(x) = [1/\Gamma(\alpha)\beta^\alpha] * x^{(\alpha - 1)} * \exp(-x/\beta), \text{ for } x > 0, \alpha, \beta > 0 \quad (3.3)$$

$$f(x) = 0, \text{ elsewhere} \quad (3.4)$$

where α, β are parameters defining the shape of the distribution

$\Gamma(\alpha)$ = gamma function of α .

The mode (most likely value) of the distribution is the value of the variable that is passed from MASBAL. Because this distribution normally has zero as its lower bound, the user must specify an "offset" (as a percentage of the mode). This offset is subtracted from the mode, and the x-axis is transformed so that the offset point is treated as zero. The scale on the transformed axis is adjusted so that the distance between the offset point and the mode is equivalent to $(\alpha - 1)\beta$, which is the distance between zero and the mode when Equation (3.3) is used as the probability density function.

7. beta - The probability density function for this distribution is

$$f(x) = [\Gamma(\alpha + \beta)/\Gamma(\alpha) \Gamma(\beta)] * x^{(\alpha - 1)} * (1 - x)^{(\beta - 1)}, \quad (3.5)$$

for $0 < x < 1$

$$f(x) = 0, \text{ elsewhere} \quad (3.6)$$

where α , β are parameters defining the shape of the distribution.

The mode (most likely value) of the distribution is the value of the variable that is passed from MASBAL. Because this distribution normally has zero as its lower bound, the user must specify an "offset" (as a percentage of the mode). This offset is subtracted from the mode, and the x-axis is transformed so that the offset point is treated as zero. The scale on the transformed axis is adjusted so that the distance between the offset point and the mode is equivalent to $(\alpha - 1)/(\alpha + \beta - 2)$, which is the distance between zero and the mode when Equation (3.5) is used as the probability density function.

8. exponential - The probability density function for this distribution is

$$f(x) = (1/\beta) * \exp(-x/\beta), \quad \text{for } x > 0, \quad (3.7)$$

$$f(x) = 0, \quad \text{elsewhere.} \quad (3.8)$$

where β is a parameter defining the shape of the distribution.

This distribution is actually a special case of the gamma distribution when $\alpha = 1$. The mode of the distribution is the value of the variable that is passed from MASBAL. According to Equation (3.7), zero is the most likely value in the distribution, so the the x-axis is transformed such that the value of the variable passed from MASBAL is treated as zero. The user must specify an "offset" that defines an x-axis transformation such that the distance between the offset point and the value of the variable passed from MASBAL is equivalent to the distance between 0 and 1 on the non-transformed axis.

9. nonsymmetrical uniform - This distribution has a rectangular probability density function, as shown in Figure 3.3. Unlike the symmetrical uniform distribution, the distance between the maximum value of the distribution and the value of the variable that is

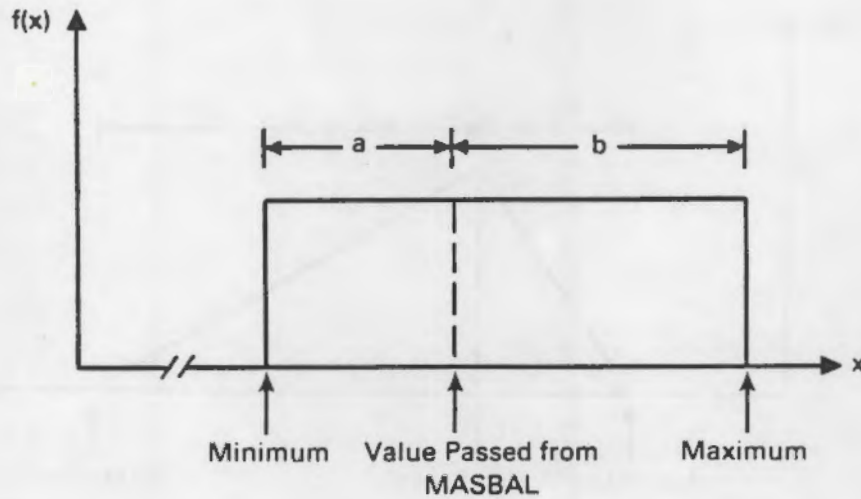


FIGURE 3.3. Probability Density Function for Nonsymmetrical Uniform Distribution

passed from MASBAL is not necessarily the same as the distance between the minimum value of the distribution and the value of the variable that is passed from MASBAL.

10. nonsymmetrical triangular - This distribution has a triangular probability density function, as shown in Figure 3.4. Unlike the symmetrical triangular distribution, the distance between the maximum value of the distribution and the value of the variable that is passed from MASBAL is not necessarily the same as the distance between the minimum value of the distribution and the value of the variable that is passed from MASBAL. The minimum and maximum value of the distribution and the value of the variable that is passed from MASBAL is not necessarily the same as the distance between the minimum value of the distribution and the value of the variable that is passed from MASBAL. The minimum and maximum values both have a probability of zero (thus defining the base of the triangle) and the value of the variable that is passed from MASBAL has the highest probability (thus forming the apex of the triangle).

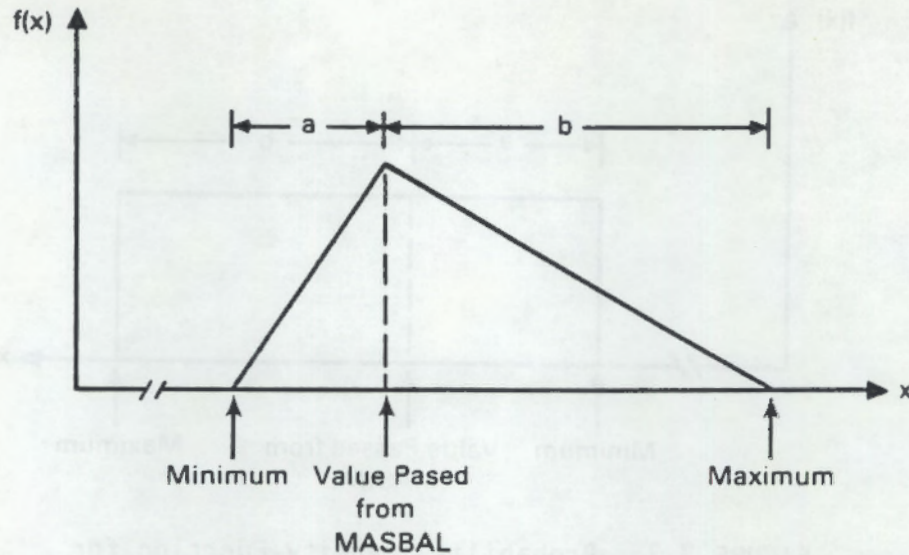


FIGURE 3.4. Probability Density Function for Nonsymmetrical Triangular Distribution

3.11.2 User-Specified Inputs

The user specifies the statistical distributions that describe each of the uncertainties in the process as well as all the parameters necessary to define these distributions. In MASBAL, the user must always specify one of the first four distributions listed in Section 3.11.1 to describe errors in process measurements. This constraint exists because it is believed that all measurement errors are characterized by symmetrical distributions (the measured value comes from a distribution having a mean equal to the true value of the measured variable). This constraint does not apply to sources of inherent variability in the system, such as the batch-to-batch variability in the composition of the feed and the variability in the amount of water added to the slurry by the steam jet (both of which contribute to the overall variability in the feed composition).

Bias in process measurements is not strictly addressed in MASBAL because it is not a random error. If a measurement is known to have bias, the bias should be removed before the measurement is entered in one of the input files.

The inputs in STOCH.DAT are described in this section. The reader is referred to Appendix A to see how the inputs are formatted in a typical STOCH.DAT file.

- TIME DISTRIBUTION - The user must choose one of the first four distributions in Section 3.11.1 for simulating errors in time measurements. A distribution is specified by entering an integer from 1 to 4. The user is limited to a choice of symmetrical distributions because it is believed that the error in measuring time will always be symmetrically distributed about the true time. If the user specifies an integer other than 1 to 4, the code will give an error message.
- TIME STANDARD DEVIATION - This specifies the "width" of the time distribution (in hours). If 1 is chosen as the distribution, the input is ignored. If 2 is chosen, the input is taken to be the standard deviation of a normal distribution that has a mean equal to the measured time. If 3 or 4 is chosen, the input is added and subtracted from the measured time to obtain the maximum and minimum of the distribution.
- FEED TANK VOLUME DISTRIBUTION - Discussion is analogous to TIME DISTRIBUTION except that this distribution is for simulating errors in measuring the level in the feed tank.
- FEED TANK VOLUME STANDARD DEVIATION - Discussion is analogous to TIME STANDARD DEVIATION except that the units are liters.
- FEED RATE DISTRIBUTION - Discussion is analogous to TIME DISTRIBUTION except that this distribution is for simulating errors in measuring the feed rate.
- FEED RATE STANDARD DEVIATION - Discussion is analogous to TIME STANDARD DEVIATION except that the units are liters per hour.
- GLASS POUR MASS DISTRIBUTION - Discussion is analogous to TIME DISTRIBUTION except that this distribution is for simulating errors in measuring the mass of glass pours.
- GLASS POUR MASS STANDARD DEVIATION - Discussion is analogous to TIME STANDARD DEVIATION except that the units are kilograms.

- GLASS FORMER ADDITION DISTRIBUTION - Discussion is analogous to TIME DISTRIBUTION except that this distribution is for simulating errors in measuring the volume of slurry added to either the feed tank or the melter.
- GLASS FORMER ADDITION STANDARD DEVIATION - Discussion is analogous to TIME STANDARD DEVIATION except that the units are liters.
- MELTER GLASS VOLUME DISTRIBUTION - Discussion is analogous to TIME DISTRIBUTION except that this distribution is for simulating errors in measuring the volume of glass in the melter.
- MELTER GLASS VOLUME STANDARD DEVIATION - Discussion is analogous to TIME STANDARD DEVIATION except that the units are liters.
- SLURRY SAMPLING ERROR - The inputs must be entered in tabular form. All alphanumeric constituent names that appear in the constituent list in DESIGN.DAT must be entered in the "Constituent" column. A distribution for each constituent must be entered in the "Dist." column, and a standard deviation for each constituent is entered in the "Std. Dev" column. The distributions are used to simulate sampling errors that occur when a slurry sample is taken (from either the makeup tank or the feed tank). The sampling errors result in sample-to-sample variation when replicate samples are taken. Each constituent must be assigned a distribution (from 1 to 4). If a constituent is left out, or if an integer other than 1 to 4 is specified for the distribution, the code will give an error message. All standard deviations should be specified as percentages of the measured values (relative percent error). If distribution 1 is specified for a constituent, the standard deviation of that constituent is ignored.
- SLURRY ANALYTICAL ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate errors in analyzing the slurry samples.

- OFF-GAS SAMPLING ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate errors that occur when off-gas samples are taken.
- OFF-GAS ANALYTICAL ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate errors in analyzing the off-gas samples.
- GLASS SAMPLING ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate errors that occur when glass samples are taken.
- GLASS ANALYTICAL ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate errors in analyzing the glass samples.
- SHIM PREPARATION ERROR - Discussion is analogous to SLURRY SAMPLING ERROR except that the distributions are used to simulate the uncertainty in knowing the composition of a slurry mixture based on a knowledge of how the slurry was prepared (i.e., knowing the amount of each ingredient that was added to the mixture).
- BATCH-TO-BATCH FEED VARIATION - The inputs must be entered in tabular form. All alphanumeric constituent names that appear in the constituent list in DESIGN.DAT must be entered in the "Constituent" column. A distribution for each constituent must be entered in the "Dist." column. The user may choose any of the ten distributions described in Section 3.11.1, except for the symmetrical uniform and symmetrical triangular distributions (these distributions can still be specified by selecting the nonsymmetrical uniform or triangular distributions and setting the distance between the maxima and the mode equal to the distance between the minima and the mode). The distributions are specified by entering any integer from 1 to 10 (except 3 or 4). The distributions are used to simulate the variation in feed composition that occurs from batch to batch when MASBAL is run in MODE 3 (or when "future" batches occur in mode 2). Values for "A",

"B", and "C" should be entered for each constituent in the appropriate column. A, B, and C are interpreted differently for different distributions. A "key" for interpretation of A, B, and C for each distribution is provided above the batch-to-batch feed variation table in STOCH.DAT (see printout in Appendix A). The key is described in greater detail here:

<u>Dist.</u>	<u>Parameters</u>
1	A, B, and C are ignored (no parameters).
2	A - standard deviation specified as a percentage of the value that is passed from MASBAL. B and C are ignored.
5	A - mean for a log-normal distribution B - standard deviation for a log-normal distribution C - offset specified as a percentage of the value that is passed from MASBAL - The offset is subtracted from the value passed from MASBAL. The resulting value is then taken as the point where the distribution first attains a probability greater than zero. The value passed from MASBAL is used as the mode of the distribution.
6	A - Value of alpha in the probability density function for a gamma distribution. B - Value of beta in the probability density function for a gamma distribution. C - Offset specified as a percentage of the value that is passed from MASBAL. The offset is subtracted from the value passed from MASBAL. The resulting value is then taken as the point where the distribution first attains a probability greater than zero. The value passed from MASBAL is used as the mode of the distribution.
7	A - Value of alpha in the probability density function for a beta distribution. B - Value of beta in the probability density function for a beta distribution. C - Offset specified as a percentage of the value that is passed from MASBAL. The offset is subtracted from the value passed from MASBAL. The resulting value is then taken as the point where the distribution first attains a probability greater than zero. The value passed from MASBAL is used as the mode of the distribution.

<u>Dist.</u>	<u>Parameters</u>
8	<p>A - Value of beta in the probability density function for a exponential distribution.</p> <p>B - Offset specified as a percentage of the value that is passed from MASBAL. The offset defines an x-axis transformation such that the distance between the offset point and the value of the variable passed from MASBAL is equivalent to the distance between 0 and 1 on the non-transformed axis (see Equation 3.7).</p> <p>C - ignored.</p>
9	<p>A - Maximum value for the uniform distribution specified as a percentage of the value that is passed from MASBAL.</p> <p>B - Minimum value for the uniform distribution specified as a percentage of the value passed from MASBAL.</p> <p>C - ignored.</p>
10	<p>A - Maximum value for the triangular distribution specified as a percentage of the value that is passed from MASBAL.</p> <p>B - Minimum value for the triangular distribution specified as a percentage of the value passed from MASBAL.</p> <p>C - ignored.</p>

- STEAM JET VOLUME CORRECTION FACTOR DISTRIBUTION - A distribution must be specified under "Dist.", and a value for A, B, and C must be specified under the appropriate letter. The distribution can be specified by entering any integer from 1 to 10, except 3 or 4. A, B, and C are interpreted differently for different distributions (see BATCH-TO-BATCH FEED VARIATION). The specified distribution is used to simulate the uncertainty in the volume correction factor for the amount of water that is added to the feed during transfer from the makeup tank to the feed tank by steam jet.



4.0 OUTPUT FILES

The primary output generated by MASBAL is the composition of the glass exiting the melter as a function of time. When the production version of MASBAL is run, the glass composition data are essentially the only output that the code produces. When the debug version is run, however, several output files are generated in addition to those generated by the production version. These files are useful for determining the exact sequence of events that occurred in the simulation and for debugging the program. The files generated by both versions are discussed in the following sections. Examples of all output files are provided in Appendix B.

4.1 OUTPUT FILES GENERATED BY PRODUCTION VERSION

Only two sets of files are generated when the production version of MASBAL is run. The first set of files provides information on the glass composition (mass fraction) in the last region of the melter as a function of time. These files have the names COMP1.OUT through COMPx.OUT, where x is a number between 1 and 20. A separate file is written for every five constituents that are specified in the model (a maximum of 20 files are created when 96 to 100 constituents are specified). Two examples of COMPx.OUT files are given in Appendix C (COMP1.OUT and COMP2.OUT). The time interval for writing the mass fractions to the files is specified by the user in the input file MODE.DAT.

The second set of output files generated by the production version of MASBAL provides information on the masses and average compositions of each glass pour. The file PORSUM.OUT gives the starting and stopping times and masses (in kilograms) of each pour. The files POUR1.OUT through POURx.OUT (where x is a number between 1 and 20) give the average mass fraction of each constituent in each of the pours. The pours are numbered for cross reference between the different files. A separate file named POURx.OUT is created for every five constituents specified in the model. Examples of PORSUM.OUT and POURx.OUT (POUR1.OUT and POUR2.OUT) are given in Appendix B.

4.2 OUTPUT FILES GENERATED BY DEBUG VERSION

When the debug version of MASBAL is run, several files are generated in addition to those generated by the production version. These files are divided into two categories: 1) those that are generated before the simulation begins, and 2) those that are generated during the simulation. All the files that fall into the first category have the extension ".ECH". The data written to these files are "echoes" of input data that are read by the PRIME subroutine and by the various subroutines that PRIME calls. All the files that are generated during the simulation have the extension ".OUT". The following list provides a brief description of the contents of each of the output files generated by the debug version of MASBAL (excluding the files that are generated by the production version):

- BATRD.ECH - Contains echoes of initial data read from the input file BATCH.DAT by the subroutine BATRD. If MASBAL is run in modes 2, the values in BATRD.ECH will differ slightly from the values in BATCH.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.
- DSNRD.ECH - Contains echoes of all the data read from the input file DESIGN.DAT by the subroutine DSNRD.
- FEEDRD.ECH - Contains echoes of initial data read from the input file FEED.DAT by the subroutine FEEDRD. If MASBAL is run in modes 2, the values in FEEDRD.ECH will differ slightly from the values in FEED.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.
- FSHRD.ECH - Contains echoes of initial data read from the input file FSHIM.DAT by the subroutine FSHRD. If MASBAL is run in modes 2, the values in FSHRD.ECH will differ slightly from the values in FSHIM.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.

- INITRD.ECH - Contains echoes of all the data read from the input file INIT.DAT by the subroutine INITRD. If MASBAL is run in modes 2 or 3, the values in INITRD.ECH will differ slightly from the values in INIT.DAT because random measurement errors will be simulated.
- MODERD.ECH - Contains echoes of all the data read from the input file MOOE.DAT by the subroutine MODERD.
- MSHRD.ECH - Contains echoes of initial data read from the input file MSHIM.DAT by the subroutine MSHRD. If MASBAL is run in modes 2, the values in MSHRD.ECH will differ slightly from the values in MSHIM.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.
- OFFRD.ECH - Contains echoes of initial data read from the input file OFFGAS.DAT by the subroutine OFFRD. If MASBAL is run in modes 2 or 3, the values in OFFRD.ECH will differ slightly from the values in OFFGAS.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.
- POURRD.ECH - Contains echoes of initial data read from the input file POUR.DAT by the subroutine POURRD. If MASBAL is run in modes 2 or 3, the values in POURRD.ECH will differ slightly from the values in POUR.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, this file is not generated.
- PRIME.ECH - If MASBAL is run in mode 3, this file contains the time at which the first glass pour is scheduled to start. If MASBAL is run in modes 1 or 2, this file is empty.
- STOCDR.ECH - Contains echoes of all the data read from the input file STOCH.DAT by the subroutine STOCDR. If MASBAL is run in mode 1, this file is not generated.
- BATCH.OUT - Contains the starting and stopping times of transfers of slurry from the makeup tank to the feed tank, and the simulated concentrations of each constituent in the feed tank after each transfer. BATCH.OUT also contains echoes of data read from the input file BATCH.DAT during the simulation. If MASBAL is run in mode 2, the

simulated times and concentrations will differ slightly from the values in BATCH.DAT because random measurement errors will be simulated. If MASBAL is run in mode 3, the times and concentrations will not be read from BATCH.DAT, but they will be generated internally by the program. In this case, BATCH.OUT will contain echoes of the internally generated times and concentrations. The concentrations written to the file will correspond to concentrations in the makeup tank, which differ from concentrations in the feed tank because water is added to the slurry during the transfer from the makeup tank to the feed tank (as a result of the steam jet).

- CHGREG.OUT - Contains the times at which the subroutine CHGREG is called and the name of the subroutine that made the call. CHGREG is called each time the melter feed rate or feed composition changes, as these changes will cause the masses of the various regions in the melter to change (assuming that the melter is not modeled as a single ideally-mixed region).
- FDRATE.OUT - Contains the times at which the melter feed rate changes and the new feed rate after each change. FDRATE.OUT also contains echoes of data read from the input file FEED.DAT during the simulation.
- OFFGAS.OUT - Contains the times at which the offgas system is sampled and the volatilization rates of each constituent, which are calculated from the offgas data. OFFGAS.OUT also contains echoes of data read from the input file OFFGAS.DAT during the simulation. When MASBAL is run in mode 3, this file is empty.
- PORHIS.OUT - Contains the times at which glass pours are started and stopped and the masses of the pours (in chronological order). Information specifying whether a glass pour was 1) scheduled from POUR.DAT, 2) scheduled as a "future pour" from within MASBAL, or 3) interrupted as a result of a low glass level in the melter is also contained in PORHIS.OUT.

- REGMAS.OUT - Contains the mass of each region in the melter as a function of time. The interval for writing the masses to the file is the same as the interval for writing mass fractions in the last region of the melter to the COMPx.OUT files (see Section 4.1). This interval is specified by the user in MODE.DAT.
- SHIMS.OUT - Contains the times at which glass formers are added to either the feed tank or the melter and the compositions of the slurries that are added. If glass formers are added to the feed tank, the composition in the feed tank immediately after the addition is written to the file. SHIMS.OUT also contains echoes of data read from the input files FSHIM.DAT and MSHIM.DAT during the simulation. When MASBAL is run in mode 3, SHIMS.OUT is empty.



5.0 EXECUTION OF MASBAL

To execute MASBAL, the SIMAN simulation language must be installed on the host computer system, and the following files must be present in the default directory:

- DMASBAL.EXE
- PMASBAL.EXE
- MASBAL.P
- The 11 input files described in Chapter 3.D.

If MASBAL is installed on a Digital Equipment Corporation VAX/VMS computer system, the VAX/VMS command files supplied with the MASBAL software package can be used to run the program. If another computer system is used, a specific set of instructions will have to be developed to properly execute the program.

MASBAL can be run in either interactive mode or batch mode. The advantage of running the program in batch mode is that once the job is submitted, the user can issue other commands or log out while the job is executing. If MASBAL is run in the interactive mode, the user will have to wait until the run completes before the terminal can be used for other commands. An advantage to running in the interactive mode is that the user will know immediately if an execution error or an error due to improper setup of the input files occurs.

Assuming that MASBAL is installed on a VAX computer, the following commands can be issued to execute the program:

- DMASBAL - to run the debug version in interactive mode
- PMASBAL - to run the production version in interactive mode
- DMASBAT - to run the debug version in batch mode
- PMASBAT - to run the production version in batch mode.

The time required to complete a run is dependent on several factors, the most important of which are the length of the simulation and the number of constituents in the simulation. The run time is almost directly proportional to the length of the simulation (doubling the simulation length will double the run time), but it is less than directly proportional to the number of constituents (doubling the number of constituents will increase the run time but not by

a factor of two). The exact time required for a run will depend on the computer system used and the number of other active processes on the system.

Regardless of whether MASBAL is run in the batch or interactive mode, the code does not prompt the user for information. All information must be present in the MASBAL input files prior to the start of the run. If the information in the input files is erroneous or inconsistent, the run will either terminate with error status or complete with results that are obviously incorrect.

6.0 TEST CASES

During the development of MASBAL, several test cases were run to test various features of the program. Some of these test cases provide excellent demonstrations of the capabilities of MASBAL.

6.1 BORON TRACER STUDIES

In one series of test cases, a step change in the concentration of boron in the feed to the melter was simulated. The step change occurred after 10 hours of operation of the melter (when a new batch of feed was transferred from the makeup tank to the feed tank). The concentration of boron in the feed tank prior to the transfer was 35 g oxide/L, corresponding to a mass fraction of B_2O_3 in the glass of 0.1. The concentration of boron in the feed tank after the transfer was 70 g oxide/L, corresponding to a mass fraction of B_2O_3 in the glass of 0.2 (the concentration of silicon in the feed tank simultaneously dropped from 175 g oxide/L to 140 g oxide/L in order to maintain constant oxide loading in the feed).

Seven cases were run in which the mixing characteristics of the melter were modeled differently. The seven variations of modeling the melter were:

1. one ideally-mixed tank
2. two ideally-mixed regions in series, with each region representing 50% of the melter volume
3. three ideally-mixed regions in series, with each region representing 33.3% of the melter volume
4. four ideally-mixed regions in series, with each region representing 25% of the melter volume
5. five ideally-mixed regions in series, with each region representing 20% of the melter volume
6. a plug flow region and an ideally-mixed region in series - The plug flow region represented 20% of the melter volume

7. a plug flow region and two ideally-mixed regions in series - The plug flow region represented 20% of the melter volume, and each of the ideally-mixed regions represented 40% of the melter volume.

The results of the seven runs are shown graphically in Figures 6.1 and 6.2. The curves show how the composition of B_2O_3 in the last region of the melter varied with time as a function of how the melter was modeled. These curves are in excellent agreement with results calculated analytically. The shapes of the curves could be altered somewhat by changing the relative volume percentages of the various regions in the melter.

These test run results imply that the parameters in MASBAL could be adjusted to fit the behavior observed in actual melter tracer studies. In this way, MASBAL could be "calibrated" to simulate a specific melter system, such as the West Valley CTS.

6.2 STARTUP FROM AN IDLING CONDITION

A series of test cases was run in which a plant startup was simulated. In all of these cases, the melter was modeled as having more than one ideally-mixed region at steady state, but the initial conditions dictated that the melter be a single ideally-mixed region at the start of the simulation. This situation corresponds to a melter that is initially idling, as it is believed that idling melters are ideally-mixed. The purpose of the runs was to test the algorithms that describe the change in mass of the various regions in the melter as a function of feed rate (see Section 2.4.3).

The output from one of the test cases is shown in Figure 6.3. In this case, the melter was modeled as having two ideally-mixed regions of equal volume at steady state. The value of β in Equation (2.7) was specified as 2.0. The curves in Figure 6.3 are in excellent agreement with the predictions of Equation (2.8), which is the analytical solution of Equation (2.7). The zig-zag appearance of the curve for the second region is a result of simulating batch glass pours. This pouring strategy causes the mass of the region to fluctuate.

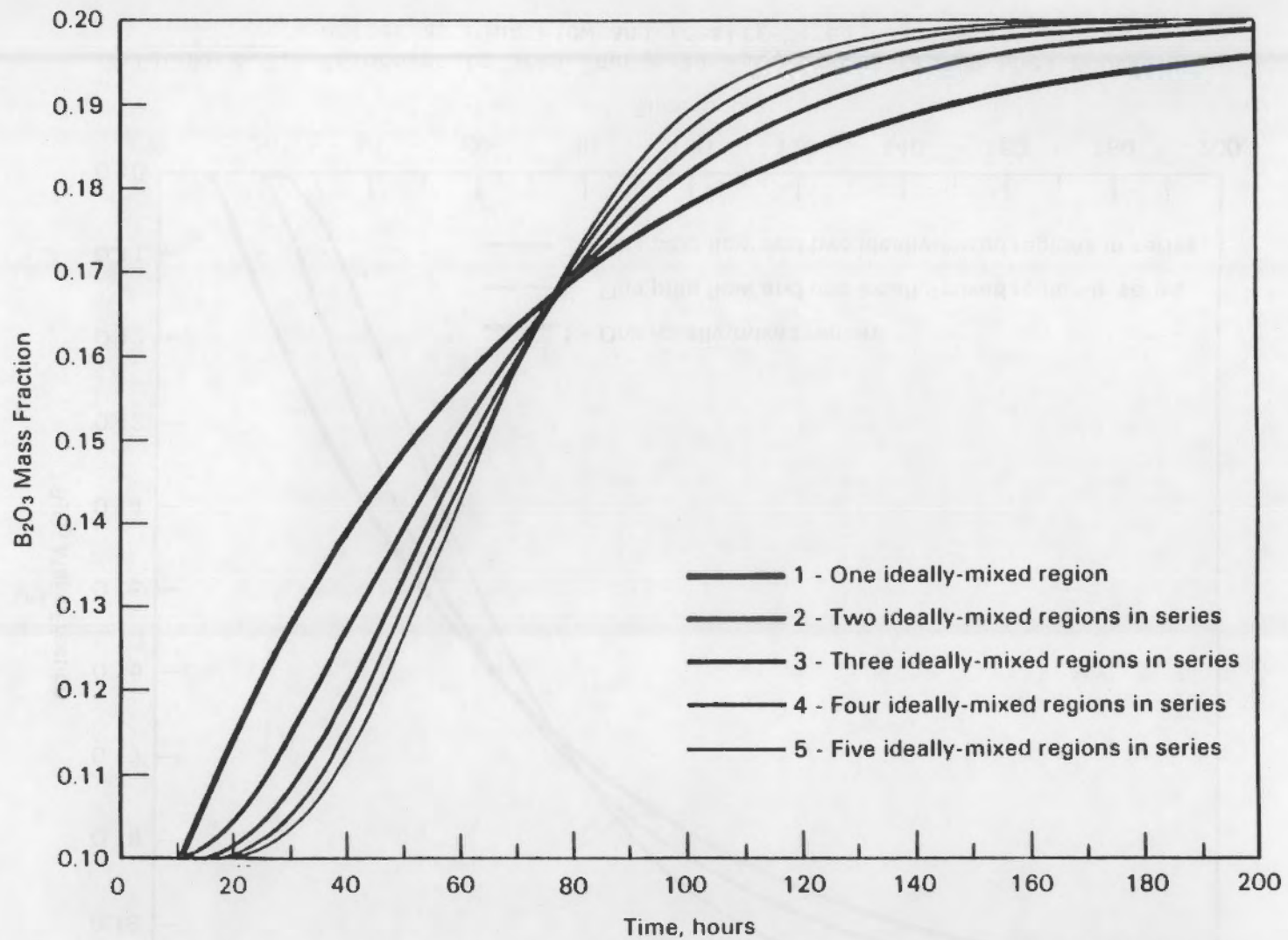


FIGURE 6.1. Responses to Step Change in B₂O₃ Concentration when Modeling Melter as Ideally-Mixed Regions in Series

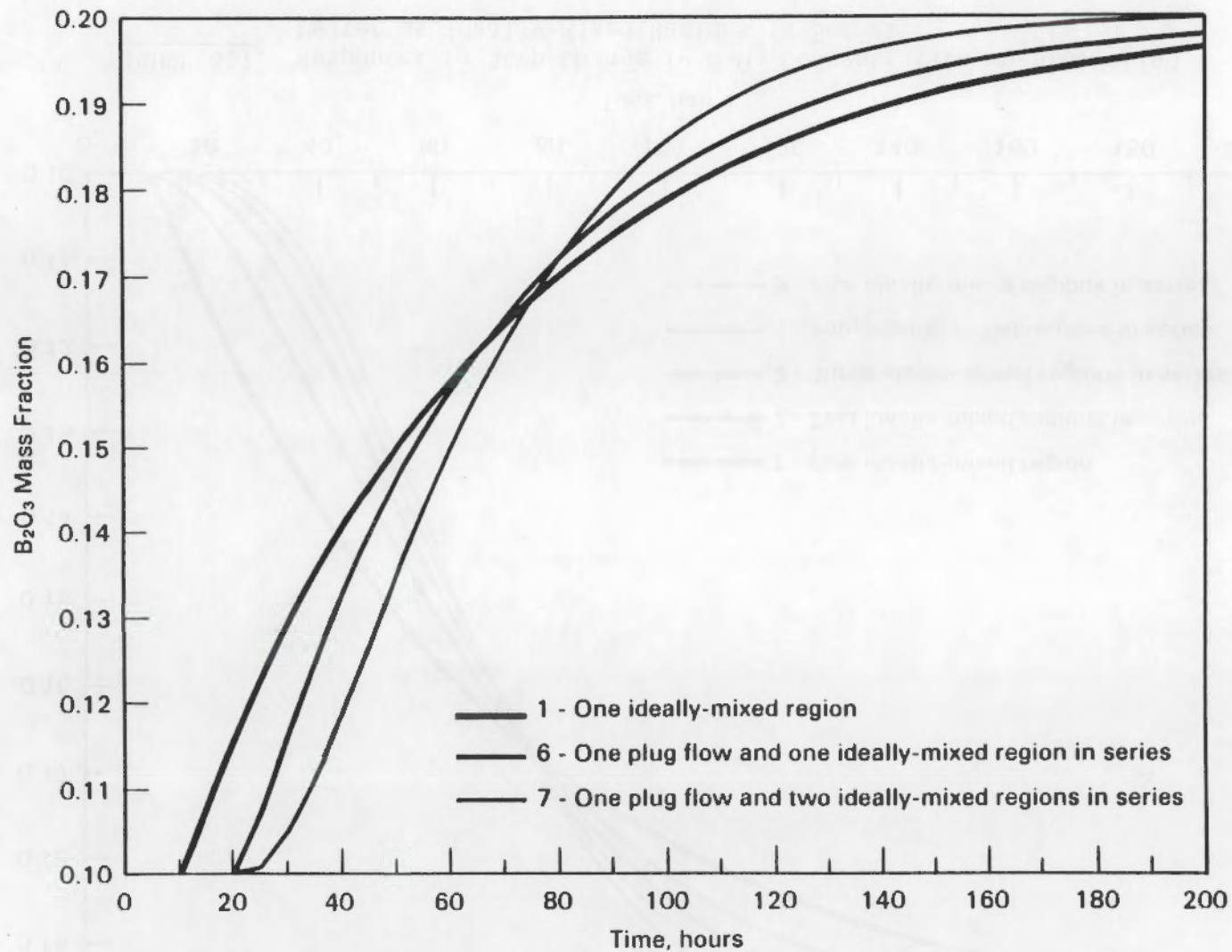


FIGURE 6.2. Responses to Step Change in B₂O₃ Concentration when Modeling Melter as Plug Flow and Ideally-Mixed Regions in Series

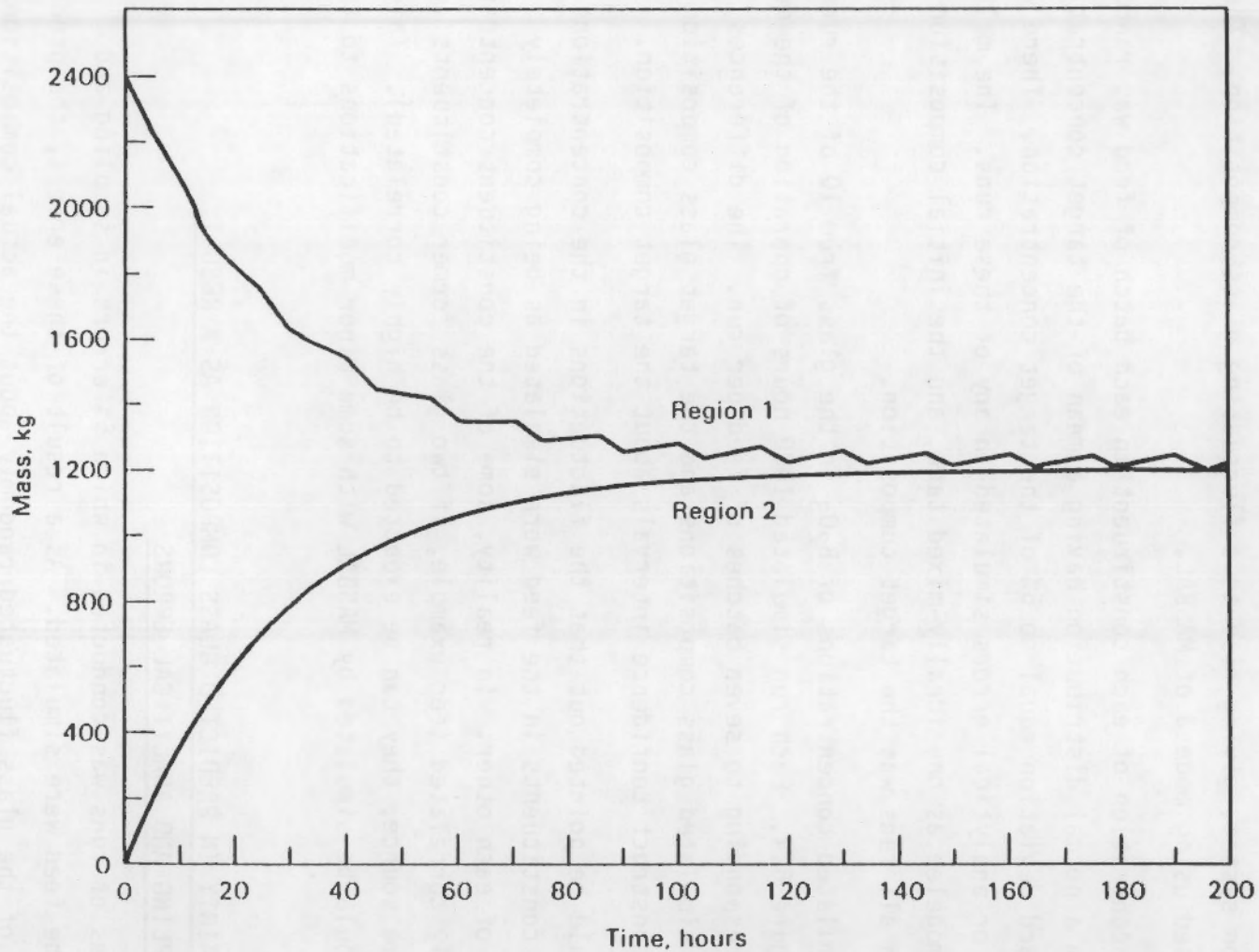


FIGURE 6.3. Change in Mass of Melter Regions when Starting from an Idling Condition (Two Ideally-Mixed Regions in Series)

6.3 VARIABILITY IN GLASS COMPOSITION AS A FUNCTION OF VARIABILITY IN FEED COMPOSITION

A series of runs was conducted in which a 5% variability in the feed composition was simulated. This variability was propagated through the simulated vitrification system, giving rise to a fluctuating glass composition. The runs were conducted using mode 3 of MASBAL.

The concentration of each constituent in each batch of feed was randomly sampled from a normal distribution having a mean of the target concentration and a standard deviation equal to 5% of the target concentration. There were no sampling or analytical errors simulated in any of these runs. The melter was always modeled as one ideally-mixed tank, and the initial composition of the glass in all runs was the target composition.

The simulated concentrations of B_2O_3 in the glass from 10 of the runs are shown in Figure 6.4. Each run simulated 1000 hours of operation of the melter system, corresponding to seven batches of feed per run. The differences between the simulated glass compositions and the target glass composition could be used to construct confidence intervals about the target composition.

It should be pointed out that the fluctuations in the concentrations of each of the constituents in the feed were simulated as being completely independent of each other. In reality, some of the constituent concentrations may be highly correlated (for example, if two glass former constituents come from the same source, they can be expected to be highly correlated). This situation could be simulated by MASBAL with some minor modifications to the program.

6.4 UNCERTAINTY IN PREDICTED GLASS COMPOSITION AS A RESULT OF SAMPLING AND ANALYTICAL ERRORS

A series of runs was conducted in which 5% errors in sampling and analyzing the feed were simulated. As a result of these errors, the predicted composition of the glass fluctuated randomly about the actual composition. The runs were conducted using mode 3 of MASBAL.

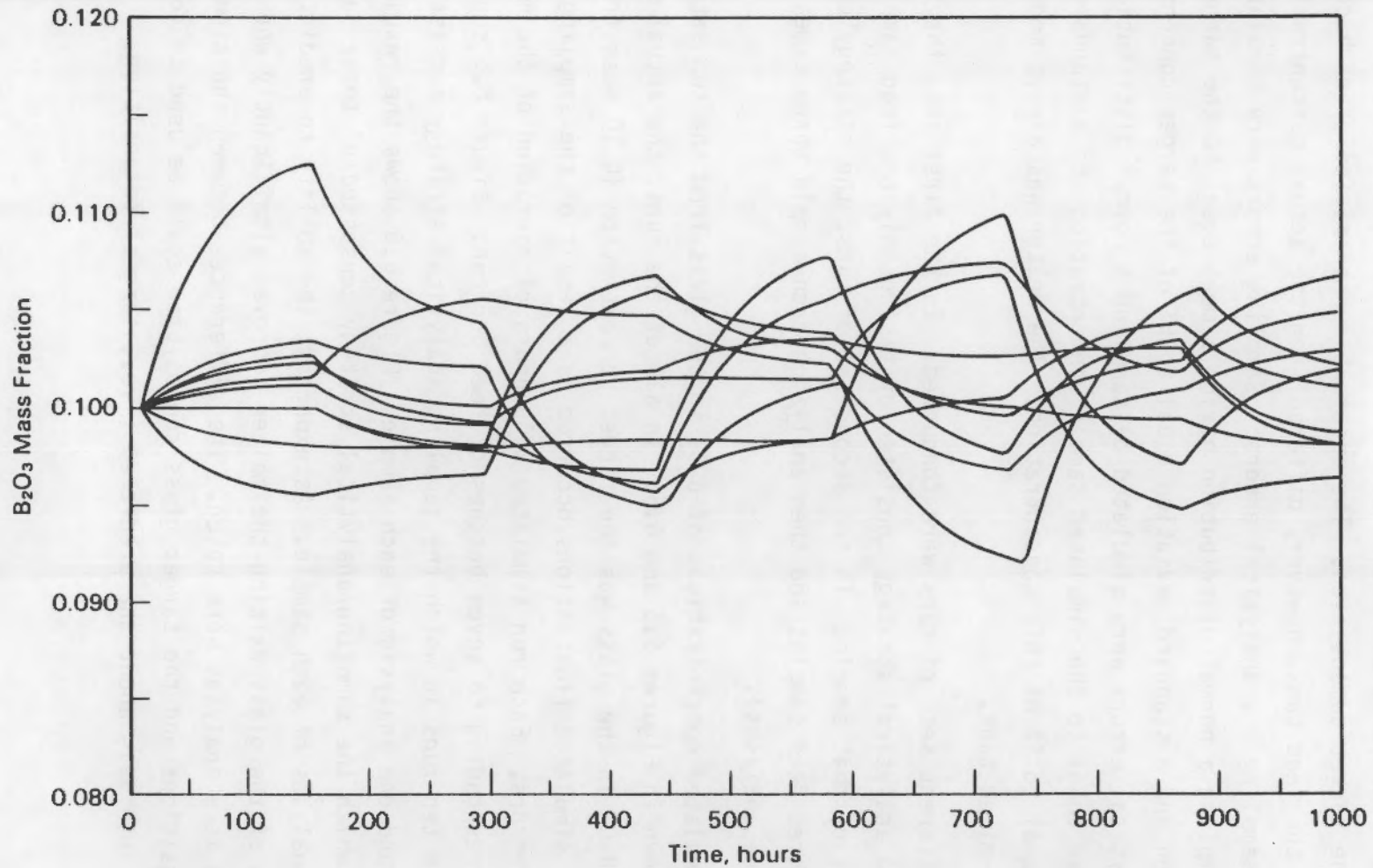


FIGURE 6.4. Variability in Glass Composition as a Result of a 5% Batch-to-Batch Variability in Feed Composition

The actual composition of each batch of feed was simulated as the target composition. Therefore, the actual composition of the glass in all runs should have been the target composition. The apparent concentration of each constituent in the feed tank, however, differed from the actual concentration because of sampling and analytical errors. Sampling errors were simulated by randomly sampling a normal distribution having a mean equal to the target concentration and a standard deviation equal to 5% of the target concentration. Analytical errors were simulated by sampling a normal distribution having a mean equal to the simulated sample concentration and a standard deviation equal to 5% of this concentration. The melter was always modeled as one ideally-mixed tank.

Two different sets of runs were conducted. In the first set, the feed sampling and analytical strategy consisted of taking only one feed sample and one analysis of that sample. In the second set of runs, the strategy consisted of taking three feed samples and then analyzing each sample three times (for a total of nine analyses).

The simulated concentrations of B_2O_3 in the glass from the two sets of runs are shown in Figures 6.5 and 6.6. In all of the runs, the actual concentration of B_2O_3 in the glass was the target concentration (0.10 mass fraction). The simulated fluctuations occurred as a result of the sampling and analytical errors. Each run simulated 1000 hours of operation of the melter system, corresponding to seven batches of feed per run. Figure 6.5 shows the results from ten runs in which the sampling/analytical strategy consisted of one sample and one analysis of each sample. Figure 6.6 shows the results from 10 runs in which the sampling/analytical strategy consisted of three samples and three analyses of each sample. As expected, the ability to predict the composition of the glass exiting the melter improved significantly when more samples and more analyses were taken. The differences between the simulated glass compositions and the target glass composition could be used to construct confidence intervals about the predicted (i.e., target) composition.

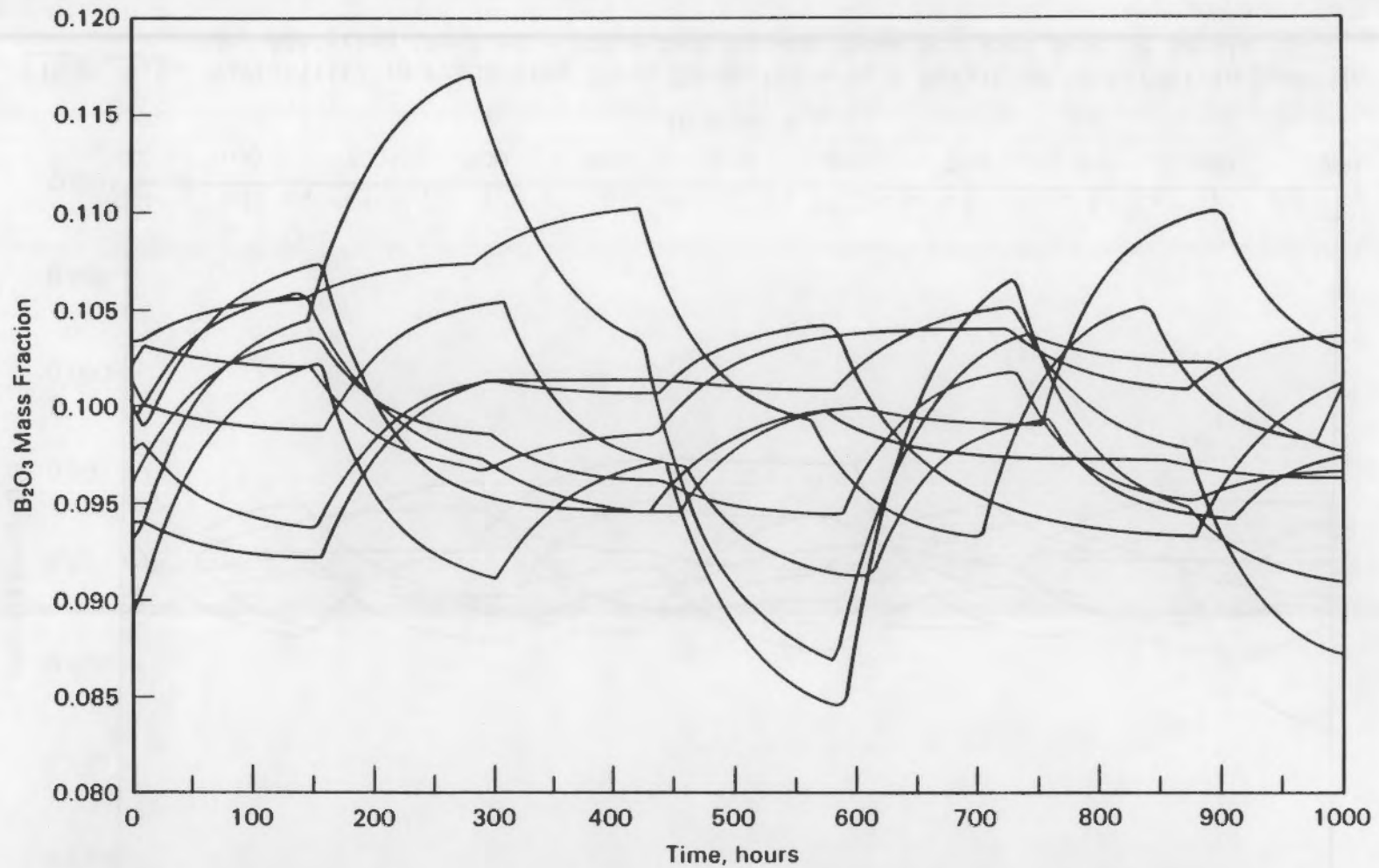


FIGURE 6.5. Variability in Predicted Glass Composition as a Result of 5% Errors in Sampling and Analyzing the Feed - One Sample and One Analysis of Each Sample

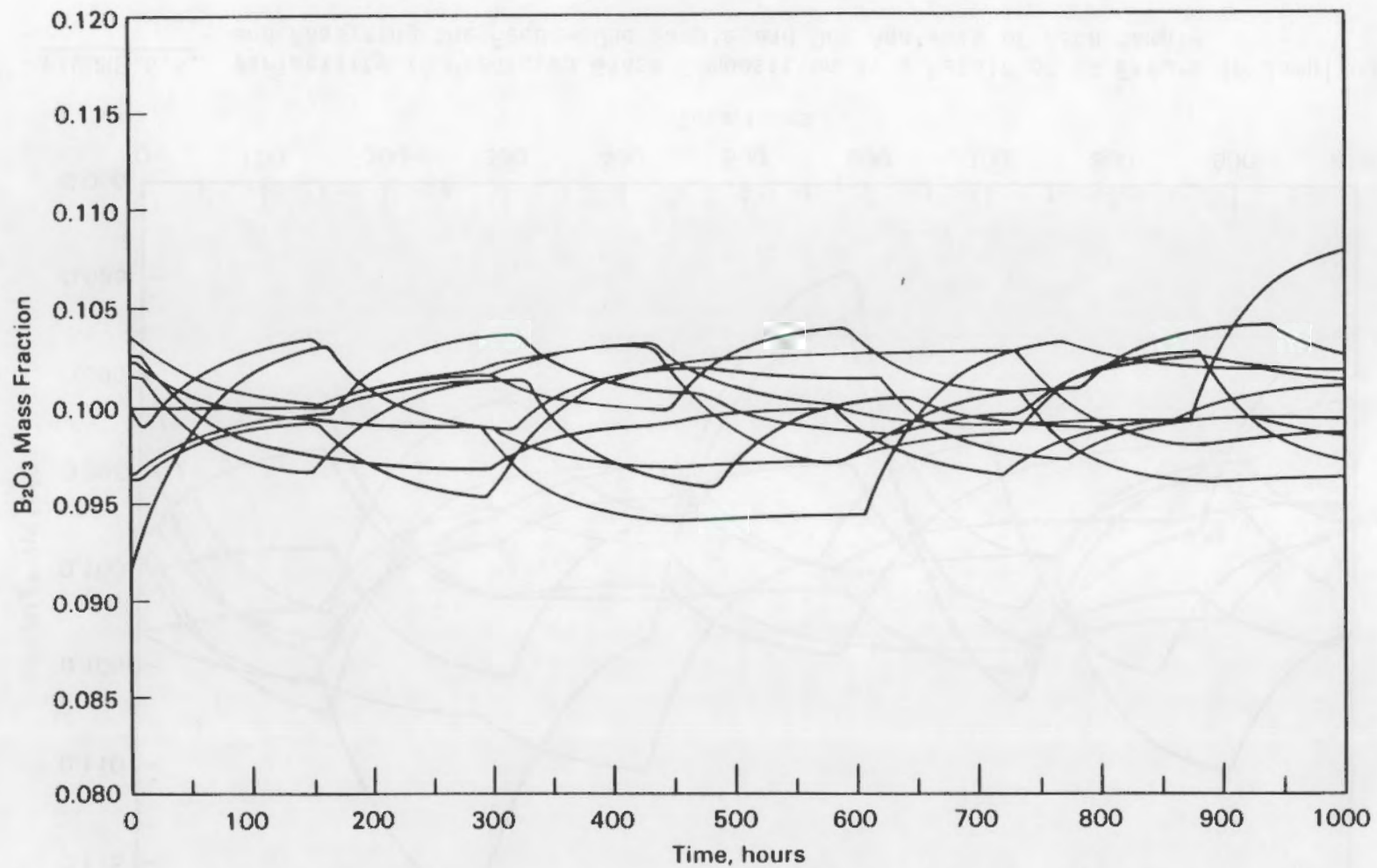


FIGURE 6.6. Variability in Predicting Glass Composition as a Result of 5% Errors in Sampling and Analyzing the Feed - Three Samples and Three Analyses of Each Sample

7.0 ACKNOWLEDGMENTS

The author would like to thank Brian Day for his help in programming MASBAL. Duane Faletti, Bill Kuhn, Joe Westsik, George Mellinger, and John Carrell all provided programmatic guidance and helpful suggestions at various times during the development of MASBAL. Ven Arakali, the principle contact at West Valley Nuclear Services, provided design input and much needed information on the West Valley vitrification system. Steve Slate provided a peer review of the report. Editorial support was provided by Ted Ceckiewicz. PNL word processing and graphics staff also assisted in preparation of the document. This report was prepared for the West Valley Support Task of the Department of Energy's Nuclear Waste Treatment Program at Pacific Northwest Laboratory.



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APPENDIX A

EXAMPLES OF INPUT FILES

- FEED TANK BATCHING INFORMATION, INCLUDING COMPOSITION IN FEED TANK AFTER EACH TRANSFER (TIMES IN HOURS, VOLUMES IN LITERS)

FOR RESULTS OF COMPOSITIONAL ANALYSES, ENTER THE NUMBER OF ANALYSES IN NO. ANAL. COLUMN. SPECIFY MULTIPLE SAMPLES BY ENTERING DUPLICATES IN THE CONSTITUENT LIST. LIST MUST END WITH "END" IN THE CONSTITUENT COLUMN.

START TIME	STOP TIME	START VOL	STOP VOL
10.0	11.42	1892.5	18925.0

RESULTS OF COMPOSITIONAL ANALYSES:

CONSTITUENT	ANAL.	G OXIDE/L		
		ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
*****	*	***.***	***.***	***.***
SI02	1	122.5	128.0	128.0
B2O3	1	70.0	65.0	65.0
NA2O	1	35.0	37.0	37.0
FE2O3	1	28.0	26.0	26.0
K2O	1	28.0	30.0	30.0
CS2O	1	1.75	1.85	1.85
SRO	1	1.75	1.65	1.65
NIO	1	14.0	15.0	15.0
ZNO	1	14.0	13.0	13.0
OTHER	1	35.0	33.0	33.0

END

START TIME	STOP TIME	START VOL	STOP VOL
153.36	154.78	1892.5	18925.0

RESULTS OF COMPOSITIONAL ANALYSES:

CONSTITUENT	ANAL.	G OXIDE/L		
		ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
*****	*	***.***	***.***	***.***
SI02	1	122.5	128.0	128.0
B2O3	1	70.0	65.0	65.0
NA2O	1	35.0	37.0	37.0
FE2O3	1	28.0	26.0	26.0
K2O	1	28.0	30.0	30.0
CS2O	1	1.75	1.85	1.85
SRO	1	1.75	1.65	1.65
NIO	1	14.0	15.0	15.0
ZNO	1	14.0	13.0	13.0
OTHER	1	35.0	33.0	33.0

END

FIGURE A.1. Input File BATCH.DAT

- TARGET COMPOSITION OF GLASS (MASS FRACTION) AND MELTER DECONTAMINATION FACTOR (DF) FOR EACH CONSTITUENT:
 MASS FRACTIONS MUST ADD UP TO 1.00 OR ERROR MESSAGE WILL RESULT
 A DF OF 1 INDICATES THAT ALL MATERIAL GOES TO THE GEP-GAS SYSTEM
 IF A DF OF ZERO IS SPECIFIED, IT WILL BE INTERPRETED AS 1.000.000
 LIST SHOULD END WITH "END" IN THE "CONSTITUENT" COLUMN

CONSTITUENT	MASS FRAC.	DECON. FACTOR
*****	*.*****	*****.***
SI02	0.45	520.0
B2O3	0.10	47.0
NA2O	0.10	280.0
FE2O3	0.08	300.0
K2O	0.08	280.0
CS2O	0.005	97.0
SRO	0.005	430.0
NIO	0.04	140.0
ZNO	0.04	560.0
OTHER	0.10	400.0
END		

***.*
 - TARGET OXIDE LOADING OF FEED (GRAMS/LITER) = 350.0

*.****
 - TARGET DENSITY OF FEED SLURRY (G/CM3) = 1.25

*.****
 - TARGET DENSITY OF GLASS (G/CM3) = 2.80

*.****
 - VOLUME CORRECTION FOR STEAM JET (L FEED/L MAKEUP) = 1.07

*****.*
 - TRANSFER RATE FROM MAKEUP TANK TO FEED TANK (L/HR) = 12000.0

*****.*
 - RATE OF ADDITION OF "SHIMS" (L/HR) = 12000.0

.
 - FEED RATE TO MELTER (L/HR) = 120.0

.
 - GLASS POURING RATE (KG/HR) = 50.4

.***
 - DURATION OF EACH GLASS POUR (HR) = 5.00

*.****
 - TIME BETWEEN POURS (STOP TO START, HR) = 1.00

*****.*
 - VOLUME IN FEED TANK AFTER FILLING (LITERS) = 18925.0

*****.*
 - VOLUME OF HEEL IN FEED TANK (LITERS) = 1892.5

****.*
 - DESIGN WORKING VOLUME OF MELTER (LITERS OF GLASS) = 860.0

*****.*

FIGURE A.2. Input File DESIGN.DAT

```

- MAXIMUM VOLUME OF GLASS ALLOWED IN MELTER (LITERS) = 1000.0
- MINIMUM VOLUME OF GLASS ALLOWED IN MELTER (LITERS) = 700.0
- PARAMETER FOR ADJUSTMENT OF TIME CONSTANT = 2.0

```

FIGURE A.2. (contd)

```

- TIME OF CHANGES IN FEED RATE AND NEW FEED RATE:
TIME (HRS)  RATE (G/HR)
*****
20.0       140.0
25.0       130.0

```

FIGURE A.3. Input File FEED.DAT

```

- TIMES AND COMPOSITIONS OF "SHIMS" ADDED TO FEED TANK
  EACH COMPOSITION SHOULD END WITH "END" IN THE "CONSTITUENT" COLUMN
TIME (HRS)  VOLUME (L)
*****
50.0       30.0
ESTIMATE OF COMPOSITION:
METHOD OF DETERMINATION (0 = BY PREP., 1 = SAMPLED) = 1
NO.
CONSTITUENT ANAL.  ANALYSIS 1  ANALYSIS 2  ANALYSIS 3
*****
SiO2          1      200.0      210.0      210.0
END

```

FIGURE A.4. Input File FSHIM.DAT

- INITIAL COMPOSITION IN FEED TANK - ENTER NUMBER OF ANALYSES IN NO. ANAL. COLUMN (MULTIPLE SAMPLES INDICATED BY DUPLICATES IN CONSTITUENT LIST). LIST MUST END WITH "END" IN CONSTITUENT COLUMN.

```

NO. ----- G OXIDE/L -----
CONSTITUENT ANAL. ANALYSIS 1 ANALYSIS 2 ANALYSIS 3
***** * ****.* ** **.* ** **.* **
SI02 1 157.5 162.5 162.5
B2O3 1 35.0 32.0 32.0
NA2O 1 35.0 38.0 38.0
FE2O3 1 28.0 25.0 25.0
K2O 1 28.0 30.0 30.0
CS2O 1 1.75 1.6 1.6
SR0 1 1.75 1.85 1.85
NIO 1 14.0 12.0 12.0
ZNO 1 14.0 16.0 16.0
OTHER 1 35.0 34.0 34.0
END

```

- INITIAL COMPOSITION IN MELTER - ENTER NUMBER OF ANALYSES IN NO. ANAL. COLUMN (MULTIPLE SAMPLES INDICATED BY DUPLICATES IN CONSTITUENT LIST). LIST MUST END WITH "END" IN CONSTITUENT COLUMN.

```

NO. ----- MASS FRACTION -----
CONSTITUENT ANAL. ANALYSIS 1 ANALYSIS 2 ANALYSIS 3
***** * *.***** *.***** *.*****
SI02 1 0.45 0.46 0.46
B2O3 1 0.10 0.09 0.09
NA2O 1 0.10 0.11 0.11
FE2O3 1 0.08 0.07 0.07
K2O 1 0.08 0.09 0.09
CS2O 1 0.005 0.004 0.004
SR0 1 0.005 0.006 0.006
NIO 1 0.04 0.035 0.035
ZNO 1 0.04 0.045 0.045
OTHER 1 0.10 0.09 0.09
END

```

- INITIAL VOLUME IN FEED TANK (LITERS) = 3092.5

- INITIAL VOLUME OF GLASS IN MELTER (LITERS) = 860.0

- INITIAL FEED RATE TO MELTER (LITERS/HR) = 120.0

- INITIAL VOLUME PERCENTAGES OF REGIONS IN MELTER:

```

REGIONS: 1 2 3 4 5
***** * ****.* ** **.* ** **.* **
0.0 100.0

```

FIGURE A.5. Input File INIT.DAT

- MOST RECENT COMPOSITION IN MAKEUP TANK (G OXIDES/L)
- 1. LIST SHOULD END WITH "END" IN THE "CONSTITUENT" COLUMN
- 2. RESULTS OF COMPOSITIONAL ANALYSES - ENTER NUMBER OF ANALYSES IN NO. ANAL. COLUMN (SPECIFY MULTIPLE SAMPLES BY ENTERING DUPLICATES IN CONSTITUENT LIST).

CONSTITUENT	NO.	----- G OXIDE/L -----		
*****	ANAL.	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
	*	***.***	***.***	***.***
SI02	1	161.5	168.5	168.5
B2O3	1	35.89	32.89	32.89
NA2O	1	35.89	37.0	37.0
FE2O3	1	28.71	30.0	30.0
K2O	1	28.71	25.0	25.0
CS2O	1	1.79	1.90	1.90
SRO	1	1.79	1.60	1.60
NIO	1	14.36	12.0	12.0
ZNO	1	29.96	31.0	31.0
OTHER	1	35.89	33.0	33.0
END				

FIGURE A.6. Input File MAKEUP.DAT


```

- MODE OF OPERATION:
  1 = DETERMINISTIC (USING PROCESS DATA)
  2 = STOCHASTIC USING PROCESS DATA
  3 = STOCHASTIC USING RANDOMLY GENERATED DATA
  *
MODE = 2

- LENGTH OF SIMULATION (HOURS) = *****
                                *****
                                200.0

- NUMBER OF REPEAT SIMULATIONS (DEFAULTS TO 1 IF MODE = 1) = ***
                                                                ***
                                                                1

- TIME INTERVAL FOR RECORDING COMPOSITION IN MELTER (HRS) = ***
                                                                ***
                                                                5.0

- IF MODE 1 OR 2 IS CHOSEN, COMPOSITION OF FUTURE
  BATCHES OF FEED:
  1 = TARGET COMPOSITION
  2 = SAME COMPOSITION AS LAST BATCH OF FEED
  *
COMPOSITION = 1

- IF 2 IS CHOSEN IN PRECEDING INPUT, HOW MANY BATCHES OF FEED
  SHOULD HAVE THIS COMPOSITION?
  **
NUMBER OF BATCHES = 10

- NUMBER OF SAMPLES OF FEED PER BATCH (CHOOSE 1 TO 5) = *
                                                                *
                                                                1

- NUMBER OF ANALYSES PER SAMPLE OF FEED (CHOOSE 1 TO 3) = *
                                                                *
                                                                1

- OPTION FOR MODELING MIXING BEHAVIOR OF MELTER:
  1 = 1 IDEALLY-MIXED REGION
  2 = 1 PLUG FLOW FOLLOWED BY 1 OR 2 IDEALLY-MIXED REGIONS IN SERIES
  3 = 2 TO 5 IDEALLY-MIXED REGIONS IN SERIES
  *
OPTION = 3

- NUMBER OF IDEALLY-MIXED REGIONS IN MELTER:
  IF OPTION 1 IS CHOSEN, INPUT IS IGNORED
  IF OPTION 2 IS CHOSEN, MUST SPECIFY 1 OR 2
  IF OPTION 3 IS CHOSEN, MUST SPECIFY 2 TO 5
  *
NUMBER = 2

- VOLUME PERCENTAGES OF REGIONS IN MELTER:
  IF OPTION 1 IS CHOSEN, INPUT IS IGNORED (100% IS ASSUMED)
  IF OPTION 2 IS CHOSEN, REGION 1 IS THE PLUG FLOW REGION
  PERCENTAGES MUST ADD UP TO 100 OR ELSE ERROR MESSAGE WILL RESULT
  IDEALLY-MIXED REGIONS SHOULD BE ORDERED FROM SMALLEST TO LARGEST

REGIONS:      1          2          3          4          5
              ***.*    ***.*    ***.*    ***.*    ***.*
              50.0      50.0

```

FIGURE A.7. Input File MODE.DAT

```

- TIMES AND COMPOSITIONS OF "SHIMS" ADDED TO MELTER
  EACH COMPOSITION SHOULD END WITH "END" IN THE "CONSTITUENT" COLUMN
TIME (HRS)  VOLUME (L)
***** **   ***** **
150.0       30.0
ESTIMATE OF COMPOSITION:
METHOD OF DETERMINATION (0 = BY PREP., 1 = SAMPLED) = 1
NO.
CONSTITUENT ANAL.  ANALYSIS 1  ANALYSIS 2  ANALYSIS 3
***** *         ***.***   ***.***   ***.***
SI02              1         200.0     210.0     210.0
END

```

FIGURE A.8. Input File MSHIM.DAT

```

- TIMES AND ANALYSES OF OFF-GAS SAMPLES
  FOR RESULTS OF COMPOSITIONAL ANALYSES, ENTER THE NUMBER OF ANALYSES
  IN NO. ANAL. COLUMN. SPECIFY MULTIPLE SAMPLES BY ENTERING DUPLICATES
  IN THE CONSTITUENT LIST. LIST MUST END WITH "END" IN THE CONSTITUENT
  COLUMN.

```

```

***** **
TIME (HRS) = 100.0
RESULTS OF COMPOSITIONAL ANALYSES:
NO.
CONSTITUENT ANAL.  ANALYSIS 1  ANALYSIS 2  ANALYSIS 3
***** *         ***** **   ***** **   ***** **
SI02              1           0.0         10.0         10.0
B2O3              1           0.0         10.0         10.0
NA2O              1           0.0         10.0         10.0
FE2O3             1           0.0         10.0         10.0
K2O               1           0.0         10.0         10.0
CS2O              1           0.0         10.0         10.0
SRO               1           0.0         10.0         10.0
NIO               1           0.0         10.0         10.0
ZNO               1           0.0         10.0         10.0
OTHER             1           0.0         10.0         10.0
END

```

```

***** **
TIME (HRS) = 200.0
RESULTS OF COMPOSITIONAL ANALYSES:
NO.
CONSTITUENT ANAL.  ANALYSIS 1  ANALYSIS 2  ANALYSIS 3
***** *         ***** **   ***** **   ***** **
SI02              1           0.0         10.0         10.0
B2O3              1           0.0         10.0         10.0
NA2O              1           0.0         10.0         10.0
FE2O3             1           0.0         10.0         10.0
K2O               1           0.0         10.0         10.0
CS2O              1           0.0         10.0         10.0
SRO               1           0.0         10.0         10.0
NIO               1           0.0         10.0         10.0
ZNO               1           0.0         10.0         10.0
OTHER             1           0.0         10.0         10.0
END

```

FIGURE A.9. Input File OFFGAS.DAT

```
- GLASS POURING DATA (TIMES IN HRS. MASS IN KG)
START TIME  STOP TIME  MASS OF POUR
*****.***  *****.***  *****.***
1.0          6.0      252.0
```

FIGURE A.10. Input File POUR.DAT

- WHEN SPECIFYING A DISTRIBUTION, USE THE FOLLOWING LEGEND:

1. CONSTANT (NO DISTRIBUTION)
2. NORMAL
3. UNIFORM (SYMMETRICAL)
4. TRIANGULAR (SYMMETRICAL)
5. LOG-NORMAL
6. GAMMA
7. BETA
8. EXPONENTIAL
9. GENERAL UNIFORM
10. GENERAL TRIANGULAR

```

TIME DISTRIBUTION (CHOOSE 1 TO 4) = 2
TIME STANDARD DEVIATION (HOURS) = 0.001

FEED TANK VOLUME DISTRIBUTION (CHOOSE 1 TO 4) = 2
FEED TANK VOLUME STANDARD DEVIATION (LITERS) = 100.0

FEED RATE DISTRIBUTION (CHOOSE 1 TO 4) = 2
FEED RATE STANDARD DEVIATION (LITERS/HR) = 5.0

GLASS POUR MASS DISTRIBUTION (CHOOSE 1 TO 4) = 2
GLASS POUR MASS STANDARD DEVIATION (KG) = 0.01

GLASS FORMER ADDITION DISTRIBUTION (CHOOSE 1 TO 4) = 2
GLASS FORMER ADDITION STANDARD DEVIATION (LITERS) = 5.0

MELTER GLASS VOLUME DISTRIBUTION (CHOOSE 1 TO 4) = 2
MELTER GLASS VOLUME STANDARD DEVIATION (LITERS) = 10.0

SLURRY SAMPLING ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)
CONSTITUENT  DIST.  STD. DEV (%)
*****      *      ***.***
SIO2         2         5.0
B2O3         2         4.0
NA2O         3         4.0
FE2O3        4         5.0
K2O          2         1.0
CS2O         2         3.0
SRO          1
NIO          2         2.223
ZNO          3         10.0
OTHER        1
END

SLURRY ANALYTICAL ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)
CONSTITUENT  DIST.  STD. DEV (%)
*****      *      ***.***
```

FIGURE A.11. Input File STOCH.DAT

SI02	2	5.0
B203	2	4.0
NA20	3	4.0
FE203	4	5.0
K20	2	1.0
CS20	2	3.0
SRO	1	
NIO	2	2.223
ZNO	3	10.0
OTHER	1	
END		

OFF-GAS SAMPLING ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)

CONSTITUENT	DIST.	STD. DEV (%)
*****	*	***.***
SI02	2	5.0
B203	2	4.0
NA20	3	4.0
FE203	4	5.0
K20	2	1.0
CS20	2	3.0
SRO	1	
NIO	2	2.223
ZNO	3	10.0
OTHER	1	
END		

OFF-GAS ANALYTICAL ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)

CONSTITUENT	DIST.	STD. DEV (%)
*****	*	***.***
SI02	2	5.0
B203	2	4.0
NA20	3	4.0
FE203	4	5.0
K20	2	1.0
CS20	2	3.0
SRO	1	
NIO	2	2.223
ZNO	3	10.0
OTHER	1	
END		

GLASS SAMPLING ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)

CONSTITUENT	DIST.	STD. DEV (%)
*****	*	***.***
SI02	2	5.0
B203	2	4.0
NA20	3	4.0
FE203	4	5.0
K20	2	1.0
CS20	2	3.0
SRO	1	
NIO	2	2.223
ZNO	3	10.0
OTHER	1	
END		

GLASS ANALYTICAL ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)

CONSTITUENT	DIST.	STD. DEV (%)
*****	*	***.***

FIGURE A.11. (contd)

```

SI02      2      5.0
B203      2      4.0
NA20      3      4.0
FE203     4      5.0
K20       2      1.0
CS20      2      3.0
SRO       1
NIO       2      2.223
ZNO       3      10.0
OTHER     1
END

```

SHIM PREPARATION ERROR (CHOOSE 1 TO 4 FOR DISTRIBUTION)

```

CONSTITUENT  DIST.  STD. DEV (%)
*****      *      ***.***
SI02         2      5.0
B203         2      4.0
NA20         3      4.0
FE203        4      5.0
K20          2      1.0
CS20         2      3.0
SRO          1
NIO          2      2.223
ZNO          3      10.0
OTHER        1
END

```

- FOR THE FOLLOWING DISTRIBUTIONS, A, B, AND C MUST BE SPECIFIED AS FOLLOWS:

DIST.	A	B	C
1	*	*	*
2	STD DEV. (%)	*	*
5	MEAN	STD DEV.	OFFSET (% OF MEAS.)
6	ALPHA	BETA	OFFSET (% OF MEAS.)
7	ALPHA	BETA	OFFSET (% OF MEAS.)
8	BETA	OFFSET (% OF MEAS.)	*
9	MAX (% OF MEAS.)	MIN (% OF MEAS.)	*
10	MAX (% OF MEAS.)	MIN (% OF MEAS.)	*

BATCH-TO-BATCH FEED VARIATION (USE ANY DISTRIBUTION EXCEPT 3 OR 4)

```

CONSTITUENT  DIST.  A      B      C
*****      **      ***.***  ***.***  ***.***
SI02         2      5.0
B203         2      4.0
NA20         5      2.0      0.5     10.0
FE203        6      2.0      1.0     10.0
K20          7      2.0      3.0     10.0
CS20         8      0.5      5.0
SRO          1
NIO         10      5.0     10.0
ZNO          9      10.0    10.0
OTHER        1
END

```

STEAM JET VOLUME CORRECTION FACTOR DISTRIBUTION -
(USE ANY DISTRIBUTION EXCEPT 3 OR 4)

```

DIST.      A      B      C
**      ***.***  ***.***  ***.***
10      15.0     10.0

```

FIGURE A.11. (contd)

```
BEGIN;  
PROJECT,MASBAL,P.W. REIMUS.11/10/66;  
DISCRETE,1000;  
CONTINUOUS,719,1250,0.0001,0.5;  
PARAMETERS:1,1.0:  
          2,1.0,1.0:  
          3,1.0,1.0,1.0;  
EVENTS:1,S(1),N,S(1931),5.0:  
       2,S(1),P,S(1932),10.0:  
       3,S(105),P,S(1933),50.0:  
       4,S(105),N,S(1934),50.0:  
       5,S(105),N,S(1935),50.0:  
       6,S(105),P,S(1936),50.0:  
REPLICATE,1,0.0,100.0;  
END;
```

FIGURE A.12. SIMAN Experiment File MASBAL.EXP

APPENDIX B

EXAMPLES OF OUTPUT FILES


```
*****
*
*           BATRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****
```

```
START TIME OF BATCH TO FEED TANK (HR) = 10.001
STOP TIME OF BATCH TO FEED TANK (HR) = 11.420
VOLUME IN FEED TANK PRIOR TO BATCH (L) = 1819.642
VOLUME IN FEED TANK AFTER BATCH (L) = 18847.949
```

FIGURE B.1. Output File BATRD.ECH

```

*****
*
*                               DSNRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

TARGET GLASS COMPOSITION AND DECON. FACTORS

CONSTITUENT	MASS FRAC.	DECON. FACTOR
SiO2	0.450000	520.00
B2O3	0.100000	47.00
Na2O	0.100000	280.00
Fe2O3	0.080000	300.00
K2O	0.080000	280.00
CS2O	0.005000	97.00
SrO	0.005000	430.00
NiO	0.040000	140.00
ZnO	0.040000	560.00
OTHER	0.100000	400.00

TARGET OXIDE LOADING OF FEED (G/L) = 350.00
 TARGET FEED DENSITY (G/CM3) = 1.2500
 TARGET GLASS DENSITY (G/CM3) = 2.8000
 VOLUME CORRECTION FOR STEAM JET (L FEED/L MAKEUP) = 1.0700
 TRANSFER RATE FROM MAKEUP TANK TO FEED TANK (L/HR) = 12000.00
 RATE OF ADDITION OF "SHIMS" (L/HR) = 12000.00
 DESIGN FEED RATE TO MELTER (L/HR) = 120.000
 DESIGN GLASS POURING RATE (KG/HR) = 50.400
 DURATION OF EACH GLASS POUR (HR) = 5.0000
 TIME BETWEEN POURS (STOP TO START, HR) = 1.0000
 VOLUME IN FEED TANK AFTER FILLING (L) = 18925.00
 VOLUME OF HEEL IN FEED TANK (L) = 1892.50
 DESIGN WORKING VOLUME OF MELTER (L) = 860.00
 MAXIMUM VOLUME OF GLASS IN MELTER (L) = 1000.00
 MINIMUM VOLUME OF GLASS IN MELTER (L) = 700.00
 PARAMETER FOR ADJUSTMENT OF TIME CONSTANT = 2.0

FIGURE B.2. Output File DSNRD.ECH

```

*****
*
*                               FEEDRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

TIME OF INITIAL FEED RATE CHANGE (HR) = 20.001
RATE AFTER CHANGE (L/HR) = 134.443

FIGURE B.3. Output File FEEDRD.ECH

```

*****
*
*                               FSHRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

TIME OF FIRST FEED SHIM = 50.001
VOLUME OF FIRST FEED SHIM = 27.803

FIGURE B.4. Output File FSHRD.ECH

```

*****
*
*                               INITRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

INITIAL FEED COMPOSITION DATA

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	157.500	162.500	162.500
B2O3	1	35.000	32.000	32.000
NA2O	1	35.000	38.000	38.000
FE2O3	1	28.000	25.000	25.000
K2O	1	28.000	30.000	30.000
CS2O	1	1.750	1.600	1.600
SRO	1	1.750	1.850	1.850
NIO	1	14.000	12.000	12.000
ZNO	1	14.000	16.000	16.000
OTHER	1	35.000	34.000	34.000
END	0	0.000	0.000	0.000

INITIAL GLASS COMPOSITION DATA

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	0.450000	0.460000	0.460000
B2O3	1	0.100000	0.090000	0.090000
NA2O	1	0.100000	0.110000	0.110000
FE2O3	1	0.080000	0.070000	0.070000
K2O	1	0.080000	0.090000	0.090000
CS2O	1	0.005000	0.004000	0.004000
SRO	1	0.005000	0.006000	0.006000
NIO	1	0.040000	0.035000	0.035000
ZNO	1	0.040000	0.045000	0.045000
OTHER	1	0.100000	0.090000	0.090000
END	0	0.000000	0.000000	0.000000

CALCULATED CONCENTRATIONS IN FEED TANK AND MELTER

CONSTITUENT	G OX/L FEED	WT. FRAC.	NSF	NAF	NSG	NAG
SI02	144.580	0.443343	1	1	1	1
B2O3	34.198	0.107373	1	1	1	1
NA2O	34.681	0.096811	1	1	1	1
FE2O3	27.770	0.078492	1	1	1	1
K2O	27.373	0.081999	1	1	1	1
CS2O	1.662	0.005090	1	1	1	1
SRO	1.750	0.005204	1	1	1	1
NIO	14.075	0.039669	1	1	1	1
ZNO	15.163	0.037935	1	1	1	1
OTHER	35.000	0.104085	1	1	1	1

FIGURE B.5. Output File INITRD.ECH

INITIAL VOLUME IN FEED TANK (L) = 3112.19
 INITIAL VOLUME IN MELTER (L) = 848.77
 INITIAL FEED RATE = 113.24
 INITIAL VOLUME % OF REGIONS IN MELTER = 0.0 100.0 0.0 0.0 0.0
 LOW LEVEL IN FEED TANK (L) = 1871.944
 HIGH LEVEL IN FEED TANK (L) = 19028.723
 HIGH LEVEL IN MELTER (GMS) = 2762984.250
 RESTART FEED LEVEL IN MELTER (GMS) = 2622984.250
 LOW LEVEL IN MELTER (GMS) = 1959675.000
 RESTART POUR LEVEL IN MELTER (GMS) = 2099675.000

FIGURE B.5. (contd)

```

*****
*
*                      MODERD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUC
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****
  
```

```

MODE = 2
LENGTH OF SIMULATION = 200.0
NUMBER OF REPEAT SIMULATIONS = 2
TIME INTERVAL FOR RECORDING COMPOSITION = 5.0
OPTION FOR FUTURE BATCHES = 1
  IF MODE = 3, OPTION SET = 1 IN PRIME
NUMBER OF BATCHES = 10
NUMBER OF SAMPLES PER BATCH = 1
NUMBER OF ANALYSES PER SAMPLE = 1
OPTION FOR MODELING MELTER = 3
  -- THE FOLLOWING WILL BE IGNORED IF OPTION = 1 --
NUMBER OF IDEALLY-MIXED REGIONS = 2
VOLUME % OF REGIONS = 50.0 50.0 0.0 0.0 0.0
  
```

FIGURE B.6. Output File MODERD.ECH

```
*****
*
*                               MSHRD.ECH FROM MASBAL                               *
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****
```

```
TIME OF FIRST MELTER SHIM = 149.999
VOLUME OF FIRST MELTER SHIM = 28.672
```

FIGURE B.7. Output File MSHRD.ECH

```

*****
*
*                               OFFRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

INITIAL DATA FROM OFF-GAS SYSTEM

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	0.0000	10.0000	10.0000
B2O3	1	0.0000	10.0000	10.0000
NA2O	1	0.0000	10.0000	10.0000
FE2O3	1	0.0000	10.0000	10.0000
K2O	1	0.0000	10.0000	10.0000
CS2O	1	0.0000	10.0000	10.0000
SR0	1	0.0000	10.0000	10.0000
NIO	1	0.0000	10.0000	10.0000
ZNO	1	0.0000	10.0000	10.0000
OTHER	1	0.0000	10.0000	10.0000
END	0	0.0000	0.0000	0.0000

TIME WHEN OFF-GAS SAMPLE WAS TAKEN (HR) = 100.001

CALCULATED VOLATILIZATION RATES

CONSTITUENT	VOLAT RATE	NSAMO	NANLO
SI02	0.0000	1	1
B2O3	0.0000	1	1
NA2O	0.0000	1	1
FE2O3	0.0000	1	1
K2O	0.0000	1	1
CS2O	0.0000	1	1
SR0	0.0000	1	1
NIO	0.0000	1	1
ZNO	0.0000	1	1
OTHER	0.0000	1	1

FIGURE B.8. Output File OFFRD.ECH

```

*****
*
*                               POURRD.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

```

TIME OF STARTING INITIAL POUR (HR) = 1.001
TIME OF STOPPING INITIAL POUR (HR) = 6.000
MASS OF INITIAL POUR (KG) = 252.003

```

FIGURE B.9. Output File POURRD.ECH

```

*****
*
*                               PRIME.ECH FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

ECHO FROM PRIME.F05 - ONLY FOR MODE 3

FIGURE B.10. Output File PRIME.ECH


```

*****
*
*                               STOCRD.ECH FROM MASEAL
*
* Title: MASEAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  18:56:06
*
*****

```

```

TIME DISTRIBUTION = 2
TIME STANDARD DEVIATION (HOURS) = 0.00100
FEED TANK VOLUME DISTRIBUTION = 2
FEED TANK VOLUME STD DEVIATION (L) = 100.000
FEED RATE DISTRIBUTION = 2
FEED RATE STD DEVIATION (L/HR) = 5.000
GLASS POUR MASS DISTRIBUTION = 2
GLASS POUR MASS STD DEVIATION (KG) = 0.010
GLASS FORMER ADDITION DISTRIBUTION = 2
GLASS FORMER ADDITION STD DEVIATION (L) = 5.000
MELTER GLASS VOLUME DISTRIBUTION = 2
MELTER GLASS VOLUME STD DEVIATION (L) = 10.000

```

SLURRY SAMPLING ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
SI02	2	5.000
B203	2	4.000
NA20	3	4.000
FE203	4	5.000
K20	2	1.000
CS20	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

SLURRY ANALYTICAL ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
SI02	2	5.000
B203	2	4.000
NA20	3	4.000
FE203	4	5.000
K20	2	1.000
CS20	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

OFF GAS SAMPLING ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
-------------	------	---------

FIGURE B.11. Output File STOCRD.ECH

SI02	2	5.000
B2O3	2	4.000
NA2O	3	4.000
FE2O3	4	5.000
K2O	2	1.000
CS2O	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

OFF GAS ANALYTICAL ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
SI02	2	5.000
B2O3	2	4.000
NA2O	3	4.000
FE2O3	4	5.000
K2O	2	1.000
CS2O	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

GLASS SAMPLING ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
SI02	2	5.000
B2O3	2	4.000
NA2O	3	4.000
FE2O3	4	5.000
K2O	2	1.000
CS2O	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

GLASS ANALYTICAL ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
SI02	2	5.000
B2O3	2	4.000
NA2O	3	4.000
FE2O3	4	5.000
K2O	2	1.000
CS2O	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

SHIM PREPARATION ERROR DIST. AND STD. DEV.

CONSTITUENT	DIST	STD DEV
-------------	------	---------

FIGURE B.11. (contd)

SI02	2	5.000
B203	2	4.000
NA20	3	4.000
FE203	4	5.000
K20	2	1.000
CS20	2	3.000
SRO	1	0.000
NIO	2	2.223
ZNO	3	10.000
OTHER	1	0.000

BATCH-TO-BATCH FEED VARIATION DIST. AND PARAMETERS

CONSTITUENT	DIST	A	B	C
SI02	2	5.000	0.000	0.000
B203	2	4.000	0.000	0.000
NA20	5	2.000	0.500	10.000
FE203	6	2.000	1.000	10.000
K20	7	2.000	3.000	10.000
CS20	8	0.500	5.000	0.000
SRO	1	0.000	0.000	0.000
NIO	10	5.000	10.000	0.000
ZNO	9	10.000	10.000	0.000
OTHER	1	0.000	0.000	0.000

STEAM JET VOL. CORRECTION DISTRIBUTION = 10
 PARAMETERS A, B, AND C = 15.000 10.000 0.000

FIGURE B.11. (contd)

```

*****
*
*                               BATCH.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

SCHEDULED BATCH

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	122.500	128.000	128.000
B2O3	1	70.000	65.000	65.000
NA2O	1	35.000	37.000	37.000
FE2O3	1	28.000	26.000	26.000
K2O	1	28.000	30.000	30.000
CS2O	1	1.750	1.850	1.850
SRO	1	1.750	1.650	1.650
NIO	1	14.000	15.000	15.000
ZNO	1	14.000	13.000	13.000
OTHER	1	35.000	33.000	33.000
END	0	0.000	0.000	0.000

DATA CAME FROM BATCH.DAT

BATCH STARTING TIME = 10.0007

ECHO NUMBER OF SAMPLES AND NUMBER OF ANALYSES

CONSTITUENT	NSAM	NANL
SI02	1	1
B2O3	1	1
NA2O	1	1
FE2O3	1	1
K2O	1	1
CS2O	1	1
SRO	1	1
NIO	1	1
ZNO	1	1
OTHER	1	1

BATCH STOPPING TIME = 11.4197

CALCULATED COMPOSITION IN FEED TANK AFTER BATCH

CONSTITUENT G OXIDE/L

FIGURE B.12. Output File BATCH.OUT

SI02	123.768
B203	57.379
NA20	36.141
FE203	27.502
K20	28.748
CS20	1.657
SRO	1.750
NIO	14.113
ZNO	13.798
OTHER	35.000

STARTING TIME FOR NEXT BATCH = 153.3606
 STOPPING TIME FOR NEXT BATCH = 154.7787
 FEED TANK VOLUME PRIOR TO NEXT BATCH (L) = 1892.50073
 FEED TANK VOLUME AFTER NEXT BATCH (L) = 18937.72461

SCHEDULED BATCH

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	122.500	128.000	128.000
B203	1	70.000	65.000	65.000
NA20	1	35.000	37.000	37.000
FE203	1	28.000	26.000	26.000
K20	1	28.000	30.000	30.000
CS20	1	1.750	1.850	1.850
SRO	1	1.750	1.650	1.650
NIO	1	14.000	15.000	15.000
ZNO	1	14.000	13.000	13.000
OTHER	1	35.000	33.000	33.000
END	0	0.000	0.000	0.000

DATA CAME FROM BATCH.DAT

BATCH STARTING TIME = 153.3606

ECHO NUMBER OF SAMPLES AND NUMBER OF ANALYSES

CONSTITUENT	NSAM	NANL
SI02	1	1
B203	1	1
NA20	1	1
FE203	1	1
K20	1	1
CS20	1	1
SRO	1	1
NIO	1	1
ZNO	1	1
OTHER	1	1

BATCH STOPPING TIME = 154.7787

CALCULATED COMPOSITION IN FEED TANK AFTER BATCH

FIGURE B.12. (contd)

CONSTITUENT	G OXIDE/L
SI02	128.627
B2O3	71.472
NA2O	32.996
FE2O3	27.761
K2O	28.466
CS2O	1.780
SRO	1.750
NIO	13.518
ZNO	14.184
OTHER	35.000

NO MORE BATCHES ARE SCHEDULED

FIGURE B.12. (contd)

```

*****
*
*                               CHGREG.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

HISTORY OF CALLS TO SUBROUTINE CHGREG

TIME	SUBROUTINE MAKING CALL
10.0110	FEDEQ
10.0207	FEDEQ
10.0221	FEDEQ
10.0132	FEDEQ
10.0221	FEDEQ
10.0378	FEDEQ
10.0457	FEDEQ
10.0802	FEDEQ
10.0850	FEDEQ
10.0536	FEDEQ
10.0850	FEDEQ
10.1160	FEDEQ
10.1314	FEDEQ
10.1993	FEDEQ
10.2088	FEDEQ
10.1469	FEDEQ
10.2088	FEDEQ
10.2508	FEDEQ
10.2718	FEDEQ
10.3640	FEDEQ
10.3769	FEDEQ
10.2928	FEDEQ
10.3769	FEDEQ
10.4503	FEDEQ
10.5576	FEDEQ
10.5726	FEDEQ
10.4747	FEDEQ
10.5726	FEDEQ
10.7684	FEDEQ
10.7847	FEDEQ
10.7847	FEDEQ
11.0059	FEDEQ
11.0243	FEDEQ
11.0243	FEDEQ
20.0005	CHFEED
24.9993	CHFEED
149.9990	MSHIM
150.0014	MSTOP
153.4856	FEDEQ
153.5481	FEDEQ
153.8221	FEDEQ
153.8606	FEDEQ
153.6106	FEDEQ
153.8606	FEDEQ
154.3231	FEDEQ
154.3606	FEDEQ
154.1106	FEDEQ
154.3606	FEDEQ

FIGURE B.13. Output File CHGREG.OUT

```

*****
*
*                               COMP 1.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

COMPOSITION IN LAST MELTER REGION (MASS FRACTION)

TIME	SI02	B203	NA2O	FE2O3	K2O
0.00	0.443343	0.107373	0.096811	0.078492	0.081999
5.00	0.443250	0.107334	0.096854	0.078520	0.081995
10.00	0.442978	0.107218	0.096983	0.078604	0.081983
15.00	0.441954	0.107722	0.097195	0.078709	0.081969
20.00	0.439571	0.109599	0.097481	0.078799	0.081960
25.00	0.435864	0.112824	0.097838	0.078871	0.081957
30.00	0.431066	0.117175	0.098247	0.078924	0.081960
35.00	0.425587	0.122255	0.098683	0.078961	0.081966
40.00	0.419675	0.127818	0.099130	0.078983	0.081975
45.00	0.413575	0.133618	0.099572	0.078991	0.081987
50.00	0.407494	0.139450	0.099999	0.078989	0.082000
55.00	0.401611	0.145136	0.100401	0.078977	0.082013
60.00	0.396063	0.150539	0.100769	0.078957	0.082024
65.00	0.390939	0.155564	0.101100	0.078932	0.082034
70.00	0.386258	0.160181	0.101396	0.078903	0.082042
75.00	0.382035	0.164369	0.101658	0.078872	0.082048
80.00	0.378262	0.168128	0.101886	0.078840	0.082054
85.00	0.374925	0.171469	0.102085	0.078809	0.082058
90.00	0.372004	0.174406	0.102256	0.078779	0.082062
95.00	0.369470	0.176964	0.102402	0.078751	0.082065
100.00	0.367272	0.179191	0.102526	0.078725	0.082067
105.00	0.365375	0.181120	0.102631	0.078701	0.082069
110.00	0.363741	0.182787	0.102720	0.078679	0.082071
115.00	0.362342	0.184220	0.102796	0.078659	0.082072
120.00	0.361148	0.185446	0.102859	0.078642	0.082073
125.00	0.360136	0.186489	0.102912	0.078626	0.082073
130.00	0.359274	0.187380	0.102956	0.078612	0.082074
135.00	0.358540	0.188141	0.102993	0.078600	0.082074
140.00	0.357918	0.188788	0.103024	0.078589	0.082074
145.00	0.357390	0.189338	0.103050	0.078579	0.082074
150.00	0.356944	0.189805	0.103072	0.078571	0.082075
155.00	0.356975	0.190092	0.103013	0.078514	0.082021
160.00	0.357080	0.190532	0.102763	0.078466	0.081944
165.00	0.357280	0.191124	0.102318	0.078421	0.081839
170.00	0.357541	0.191806	0.101750	0.078381	0.081717
175.00	0.357838	0.192532	0.101110	0.078344	0.081587
180.00	0.358152	0.193267	0.100439	0.078312	0.081456
185.00	0.358466	0.193986	0.099768	0.078283	0.081327
190.00	0.358774	0.194677	0.099113	0.078257	0.081203
195.00	0.359070	0.195329	0.098486	0.078234	0.081085
200.00	0.359349	0.195938	0.097895	0.078214	0.080976

FIGURE B.14. Output File COMP 1.OUT


```

*****
*
*                               COMP 2.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  FAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

COMPOSITION IN LAST MELTER REGION (MASS FRACTION)

TIME	CS20	SRO	NIO	ZNO	OTHER
0.00	0.005090	0.005204	0.039669	0.037935	0.104085
5.00	0.005089	0.005204	0.039684	0.037985	0.104085
10.00	0.005086	0.005204	0.039729	0.038131	0.104085
15.00	0.005079	0.005203	0.039790	0.038325	0.104054
20.00	0.005068	0.005198	0.039852	0.038512	0.103960
25.00	0.005051	0.005190	0.039914	0.038688	0.103802
30.00	0.005031	0.005180	0.039974	0.038849	0.103593
35.00	0.005009	0.005167	0.040030	0.038991	0.103350
40.00	0.004985	0.005154	0.040082	0.039114	0.103085
45.00	0.004961	0.005140	0.040128	0.039217	0.102810
50.00	0.004937	0.005127	0.040168	0.039302	0.102534
55.00	0.004914	0.005113	0.040202	0.039369	0.102263
60.00	0.004893	0.005100	0.040230	0.039420	0.102004
65.00	0.004873	0.005088	0.040252	0.039457	0.101761
70.00	0.004854	0.005077	0.040270	0.039483	0.101537
75.00	0.004838	0.005067	0.040283	0.039500	0.101332
80.00	0.004823	0.005057	0.040293	0.039509	0.101147
85.00	0.004810	0.005049	0.040300	0.039513	0.100981
90.00	0.004798	0.005042	0.040305	0.039513	0.100835
95.00	0.004788	0.005035	0.040308	0.039509	0.100708
100.00	0.004780	0.005030	0.040310	0.039504	0.100596
105.00	0.004772	0.005025	0.040311	0.039497	0.100499
110.00	0.004766	0.005021	0.040311	0.039490	0.100415
115.00	0.004760	0.005017	0.040311	0.039482	0.100342
120.00	0.004755	0.005014	0.040310	0.039474	0.100280
125.00	0.004751	0.005011	0.040309	0.039466	0.100227
130.00	0.004748	0.005009	0.040308	0.039459	0.100181
135.00	0.004745	0.005007	0.040307	0.039452	0.100142
140.00	0.004743	0.005005	0.040305	0.039445	0.100109
145.00	0.004741	0.005004	0.040304	0.039440	0.100080
150.00	0.004739	0.005003	0.040303	0.039434	0.100056
155.00	0.004735	0.004999	0.040274	0.039406	0.099972
160.00	0.004738	0.004994	0.040208	0.039395	0.099881
165.00	0.004747	0.004989	0.040102	0.039402	0.099778
170.00	0.004760	0.004984	0.039972	0.039419	0.099670
175.00	0.004776	0.004978	0.039828	0.039445	0.099561
180.00	0.004794	0.004973	0.039679	0.039474	0.099455
185.00	0.004811	0.004968	0.039531	0.039506	0.099354
190.00	0.004829	0.004963	0.039387	0.039539	0.099259
195.00	0.004846	0.004959	0.039250	0.039571	0.099170
200.00	0.004862	0.004954	0.039121	0.039602	0.099089

FIGURE B.15. Output File COMP 2.OUT

```
*****
*
*                               FDRATE.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****
```

```
TIME OF FEED RATE CHANGE =    20.0005
NEW FEED RATE (L/HR) =    134.4433

TIME OF FEED RATE CHANGE =    24.9993
NEW FEED RATE (L/HR) =    120.3613
```

FIGURE B.16. Output File FDRATE.OUT

```

*****
*
*                               OFFGAS.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

NEW SET OF OFF-GAS DATA

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	0.0000	10.0000	10.0000
B203	1	0.0000	10.0000	10.0000
NA20	1	0.0000	10.0000	10.0000
FE203	1	0.0000	10.0000	10.0000
K20	1	0.0000	10.0000	10.0000
CS20	1	0.0000	10.0000	10.0000
SRO	1	0.0000	10.0000	10.0000
NIO	1	0.0000	10.0000	10.0000
ZNO	1	0.0000	10.0000	10.0000
OTHER	1	0.0000	10.0000	10.0000
END	0	0.0000	0.0000	0.0000

TIME UNTIL THE NEXT OFF-GAS SAMPLING = 200.0002

CALCULATED VOLATILIZATION RATES UNTIL NEXT SAMPLE

CONSTITUENT	VOLAT. RATE
SI02	0.0000
B203	0.0000
NA20	0.0000
FE203	0.0000
K20	0.0000
CS20	0.0000
SRO	0.0000
NIO	0.0000
ZNO	0.0000
OTHER	0.0000

FIGURE B.17. Output File OFFGAS.OUT

```

*****
*
*                               PORHIS.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

```

START TIME FOR SCHEDULED POUR = 1.0014
STOP TIME FOR SCHEDULED POUR = 6.0004

```

```

START TIME FOR FUTURE POUR = 7.0004
MASS OF POUR (KG) = 252.0108
DURATION OF POUR (HR) = 5.0008
STOP TIME FOR FUTURE POUR = 12.0012
TIME UNTIL NEXT POUR = 0.9996

```

```

START TIME FOR FUTURE POUR = 13.0009
MASS OF POUR (KG) = 251.9889
DURATION OF POUR (HR) = 5.0008
STOP TIME FOR FUTURE POUR = 18.0016
TIME UNTIL NEXT POUR = 0.9992

```

```

START TIME FOR FUTURE POUR = 19.0008
MASS OF POUR (KG) = 251.9958
DURATION OF POUR (HR) = 4.9995
STOP TIME FOR FUTURE POUR = 24.0003
TIME UNTIL NEXT POUR = 1.0002

```

```

START TIME FOR FUTURE POUR = 25.0005
MASS OF POUR (KG) = 252.0048
DURATION OF POUR (HR) = 4.9996
STOP TIME FOR FUTURE POUR = 30.0001
TIME UNTIL NEXT POUR = 0.9987

```

```

START TIME FOR FUTURE POUR = 30.9988
MASS OF POUR (KG) = 252.0033
DURATION OF POUR (HR) = 4.9995
STOP TIME FOR FUTURE POUR = 35.9983
TIME UNTIL NEXT POUR = 1.0011

```

```

START TIME FOR FUTURE POUR = 36.9994
MASS OF POUR (KG) = 252.0096
DURATION OF POUR (HR) = 4.9995
STOP TIME FOR FUTURE POUR = 41.9989
TIME UNTIL NEXT POUR = 0.9988

```

```

START TIME FOR FUTURE POUR = 42.9977
MASS OF POUR (KG) = 251.9967
DURATION OF POUR (HR) = 4.9976
STOP TIME FOR FUTURE POUR = 47.9953
TIME UNTIL NEXT POUR = 1.0012

```

```

START TIME FOR FUTURE POUR = 48.9965

```

FIGURE B.18. Output File PORHIS.OUT

MASS OF POUR (KG) = 251.9946
 DURATION OF POUR (HR) = 4.9981
 STOP TIME FOR FUTURE POUR = 53.9946
 TIME UNTIL NEXT POUR = 0.9997

START TIME FOR FUTURE POUR = 54.9943
 MASS OF POUR (KG) = 252.0115
 DURATION OF POUR (HR) = 5.0012
 STOP TIME FOR FUTURE POUR = 59.9955
 TIME UNTIL NEXT POUR = 0.9990

START TIME FOR FUTURE POUR = 60.9945
 MASS OF POUR (KG) = 252.0134
 DURATION OF POUR (HR) = 4.9994
 STOP TIME FOR FUTURE POUR = 65.9939
 TIME UNTIL NEXT POUR = 1.0005

START TIME FOR FUTURE POUR = 66.9944
 MASS OF POUR (KG) = 252.0006
 DURATION OF POUR (HR) = 4.9996
 STOP TIME FOR FUTURE POUR = 71.9940
 TIME UNTIL NEXT POUR = 1.0005

START TIME FOR FUTURE POUR = 72.9944
 MASS OF POUR (KG) = 252.0059
 DURATION OF POUR (HR) = 4.9996
 STOP TIME FOR FUTURE POUR = 77.9940
 TIME UNTIL NEXT POUR = 0.9980

START TIME FOR FUTURE POUR = 78.9921
 MASS OF POUR (KG) = 252.0051
 DURATION OF POUR (HR) = 4.9999
 STOP TIME FOR FUTURE POUR = 83.9920
 TIME UNTIL NEXT POUR = 1.0003

START TIME FOR FUTURE POUR = 84.9923
 MASS OF POUR (KG) = 251.9810
 DURATION OF POUR (HR) = 4.9986
 STOP TIME FOR FUTURE POUR = 89.9909
 TIME UNTIL NEXT POUR = 1.0010

START TIME FOR FUTURE POUR = 90.9920
 MASS OF POUR (KG) = 252.0044
 DURATION OF POUR (HR) = 5.0006
 STOP TIME FOR FUTURE POUR = 95.9926
 TIME UNTIL NEXT POUR = 0.9993

START TIME FOR FUTURE POUR = 96.9918
 MASS OF POUR (KG) = 251.9803
 DURATION OF POUR (HR) = 4.9998
 STOP TIME FOR FUTURE POUR = 101.9917
 TIME UNTIL NEXT POUR = 1.0013

START TIME FOR FUTURE POUR = 102.9930
 MASS OF POUR (KG) = 252.0029
 DURATION OF POUR (HR) = 5.0001
 STOP TIME FOR FUTURE POUR = 107.9931
 TIME UNTIL NEXT POUR = 1.0009

START TIME FOR FUTURE POUR = 108.9940

FIGURE B.18. (contd)

MASS OF POUR (KG) = 251.9954
 DURATION OF POUR (HR) = 5.0009
 STOP TIME FOR FUTURE POUR = 113.9949
 TIME UNTIL NEXT POUR = 1.0001

START TIME FOR FUTURE POUR = 114.9949
 MASS OF POUR (KG) = 251.9905
 DURATION OF POUR (HR) = 4.9994
 STOP TIME FOR FUTURE POUR = 119.9943
 TIME UNTIL NEXT POUR = 0.9993

START TIME FOR FUTURE POUR = 120.9936
 MASS OF POUR (KG) = 252.0186
 DURATION OF POUR (HR) = 4.9996
 STOP TIME FOR FUTURE POUR = 125.9932
 TIME UNTIL NEXT POUR = 1.0002

START TIME FOR FUTURE POUR = 126.9934
 MASS OF POUR (KG) = 251.9928
 DURATION OF POUR (HR) = 5.0014
 STOP TIME FOR FUTURE POUR = 131.9948
 TIME UNTIL NEXT POUR = 0.9989

START TIME FOR FUTURE POUR = 132.9937
 MASS OF POUR (KG) = 252.0075
 DURATION OF POUR (HR) = 5.0007
 STOP TIME FOR FUTURE POUR = 137.9944
 TIME UNTIL NEXT POUR = 1.0005

START TIME FOR FUTURE POUR = 138.9950
 MASS OF POUR (KG) = 252.0073
 DURATION OF POUR (HR) = 4.9996
 STOP TIME FOR FUTURE POUR = 143.9945
 TIME UNTIL NEXT POUR = 1.0000

START TIME FOR FUTURE POUR = 144.9945
 MASS OF POUR (KG) = 252.0061
 DURATION OF POUR (HR) = 4.9998
 STOP TIME FOR FUTURE POUR = 149.9943
 TIME UNTIL NEXT POUR = 1.0016

START TIME FOR FUTURE POUR = 150.9959
 MASS OF POUR (KG) = 252.0030
 DURATION OF POUR (HR) = 4.9993
 STOP TIME FOR FUTURE POUR = 155.9951
 TIME UNTIL NEXT POUR = 1.0009

START TIME FOR FUTURE POUR = 156.9961
 MASS OF POUR (KG) = 251.9928
 DURATION OF POUR (HR) = 4.9996
 STOP TIME FOR FUTURE POUR = 161.9957
 TIME UNTIL NEXT POUR = 1.0006

START TIME FOR FUTURE POUR = 162.9963
 MASS OF POUR (KG) = 251.9989
 DURATION OF POUR (HR) = 5.0005
 STOP TIME FOR FUTURE POUR = 167.9968
 TIME UNTIL NEXT POUR = 0.9987

START TIME FOR FUTURE POUR = 168.9955

FIGURE B.18. (contd)

MASS OF POUR (KG) = 252.0044
DURATION OF POUR (HR) = 5.0002
STOP TIME FOR FUTURE POUR = 173.9957
TIME UNTIL NEXT POUR = 1.0004

START TIME FOR FUTURE POUR = 174.9961
MASS OF POUR (KG) = 251.9976
DURATION OF POUR (HR) = 5.0011
STOP TIME FOR FUTURE POUR = 179.9972
TIME UNTIL NEXT POUR = 0.9996

START TIME FOR FUTURE POUR = 180.9968
MASS OF POUR (KG) = 251.9992
DURATION OF POUR (HR) = 4.9994
STOP TIME FOR FUTURE POUR = 185.9962
TIME UNTIL NEXT POUR = 1.0011

START TIME FOR FUTURE POUR = 186.9973
MASS OF POUR (KG) = 251.9885
DURATION OF POUR (HR) = 4.9974
STOP TIME FOR FUTURE POUR = 191.9947
TIME UNTIL NEXT POUR = 1.0000

START TIME FOR FUTURE POUR = 192.9947
MASS OF POUR (KG) = 251.9959
DURATION OF POUR (HR) = 4.9999
STOP TIME FOR FUTURE POUR = 197.9946
TIME UNTIL NEXT POUR = 0.9994

START TIME FOR FUTURE POUR = 198.9940
MASS OF POUR (KG) = 251.9893
DURATION OF POUR (HR) = 5.0000

FIGURE B.18. (contd)

```

*****
*
*           PORSUM.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

CANISTER POURING SUMMARY - TIMES AND MASSES OF POURS

TIMES ARE HOURS SINCE START OF SIMULATION

NUMBER	START TIME	STOP TIME	MASS (KG)
1	1.0014	6.0004	252.00288
2	7.0004	12.0012	252.01086
3	13.0009	18.0016	251.98894
4	19.0008	24.0003	251.99567
5	25.0005	30.0001	252.00479
6	30.9988	35.9983	252.00331
7	36.9994	41.9989	252.00935
8	42.9977	47.9953	251.99678
9	48.9965	53.9946	251.99486
10	54.9943	59.9955	252.01167
11	60.9945	65.9939	252.01314
12	66.9944	71.9940	252.00110
13	72.9944	77.9940	252.00560
14	78.9921	83.9920	252.00526
15	84.9923	89.9909	251.98132
16	90.9920	95.9926	252.00400
17	96.9918	101.9917	251.98018
18	102.9930	107.9931	252.00270
19	108.9940	113.9949	251.99545
20	114.9949	119.9943	251.99037
21	120.9936	125.9932	252.01865
22	126.9934	131.9948	251.99257
23	132.9937	137.9944	252.00746
24	138.9950	143.9945	252.00748
25	144.9945	149.9943	252.00635
26	150.9959	155.9951	252.00337
27	156.9961	161.9957	251.99321
28	162.9963	167.9968	251.99811
29	168.9955	173.9957	252.00433
30	174.9961	179.9972	251.99838
31	180.9968	185.9962	251.99843
32	186.9973	191.9947	251.98882
33	192.9947	197.9946	251.99617

FIGURE B.19. Output File PORSUM.OUT


```

*****
*
*                               POUR 1.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

COMPOSITION OF BATCH GLASS POURS (MASS FRACTION)

NUMBER	SI02	B203	NA2O	FE2O3	K2O
1	0.443290	0.107350	0.096836	0.078508	0.081997
2	0.442995	0.107242	0.096970	0.078595	0.081984
3	0.441716	0.107908	0.097224	0.078718	0.081968
4	0.438546	0.110478	0.097583	0.078822	0.081959
5	0.433546	0.114916	0.098039	0.078899	0.081958
6	0.427275	0.120685	0.098551	0.078951	0.081964
7	0.420267	0.127260	0.099085	0.078981	0.081974
8	0.412964	0.134204	0.099615	0.078991	0.081988
9	0.405721	0.141160	0.100121	0.078986	0.082004
10	0.398828	0.147843	0.100586	0.078968	0.082019
11	0.392463	0.154068	0.101002	0.078940	0.082031
12	0.386727	0.159718	0.101367	0.078906	0.082041
13	0.381656	0.164746	0.101681	0.078869	0.082049
14	0.377242	0.169149	0.101947	0.078831	0.082055
15	0.373446	0.172955	0.102172	0.078794	0.082060
16	0.370216	0.176210	0.102359	0.078760	0.082064
17	0.367492	0.178967	0.102513	0.078728	0.082067
18	0.365211	0.181287	0.102640	0.078699	0.082069
19	0.363310	0.183228	0.102744	0.078673	0.082071
20	0.361734	0.184844	0.102828	0.078650	0.082072
21	0.360432	0.186184	0.102896	0.078631	0.082073
22	0.359359	0.187292	0.102952	0.078613	0.082074
23	0.358478	0.188206	0.102996	0.078598	0.082074
24	0.357755	0.188958	0.103032	0.078586	0.082074
25	0.357162	0.189576	0.103061	0.078575	0.082074
26	0.356969	0.190004	0.103032	0.078530	0.082037
27	0.357068	0.190487	0.102789	0.078471	0.081952
28	0.357306	0.191193	0.102261	0.078417	0.081827
29	0.357628	0.192021	0.101562	0.078370	0.081679
30	0.357993	0.192897	0.100778	0.078328	0.081522
31	0.358371	0.193770	0.099971	0.078291	0.081365
32	0.358744	0.194607	0.099179	0.078260	0.081215
33	0.359098	0.195390	0.098426	0.078232	0.081074

FIGURE B.20. Output File POUR 1.OUT

```

*****
*
*           POUR 2.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

COMPOSITION OF BATCH GLASS FOURS (MASS FRACTION)

NUMBER	CS2O	SR0	NIO	ZNO	OTHER
1	0.005089	0.005204	0.039678	0.037964	0.104085
2	0.005086	0.005204	0.039724	0.038115	0.104084
3	0.005078	0.005202	0.039796	0.038344	0.104045
4	0.005063	0.005196	0.039871	0.038566	0.103916
5	0.005042	0.005185	0.039944	0.038770	0.103701
6	0.005016	0.005171	0.040014	0.038950	0.103425
7	0.004988	0.005156	0.040077	0.039102	0.103111
8	0.004959	0.005139	0.040132	0.039226	0.102782
9	0.004930	0.005123	0.040179	0.039323	0.102452
10	0.004903	0.005107	0.040217	0.039396	0.102134
11	0.004878	0.005092	0.040246	0.039447	0.101834
12	0.004856	0.005078	0.040268	0.039481	0.101559
13	0.004836	0.005066	0.040284	0.039501	0.101313
14	0.004819	0.005055	0.040295	0.039511	0.101096
15	0.004804	0.005045	0.040303	0.039513	0.100907
16	0.004791	0.005037	0.040307	0.039510	0.100745
17	0.004780	0.005030	0.040310	0.039504	0.100607
18	0.004772	0.005025	0.040311	0.039496	0.100491
19	0.004764	0.005020	0.040311	0.039487	0.100392
20	0.004758	0.005016	0.040310	0.039478	0.100310
21	0.004753	0.005012	0.040309	0.039468	0.100242
22	0.004748	0.005009	0.040308	0.039460	0.100185
23	0.004745	0.005007	0.040307	0.039451	0.100139
24	0.004742	0.005005	0.040305	0.039444	0.100100
25	0.004740	0.005003	0.040304	0.039437	0.100068
26	0.004736	0.005000	0.040283	0.039413	0.099996
27	0.004737	0.004995	0.040215	0.039396	0.099890
28	0.004748	0.004988	0.040089	0.039404	0.099767
29	0.004765	0.004982	0.039930	0.039427	0.099638
30	0.004785	0.004975	0.039754	0.039459	0.099508
31	0.004806	0.004969	0.039575	0.039496	0.099384
32	0.004827	0.004963	0.039401	0.039535	0.099268
33	0.004848	0.004958	0.039237	0.039574	0.099162

FIGURE B.21. Output File POUR 2.OUT

```

*****
*
*                               REGMAS.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

MASS OF ALL REGIONS IN MELTER (GMS)

TIME	REGION 1	REGION 2	REGION 3	REGION 4	REGION 5
0.00	0.00	0.00	0.00	0.00	2376564.50
5.00	174713.23	0.00	0.00	0.00	2190672.00
10.00	321462.81	0.00	0.00	0.00	2032723.50
15.00	451275.03	0.00	0.00	0.00	1899048.13
20.00	560574.31	0.00	0.00	0.00	1786228.88
25.00	686656.50	0.00	0.00	0.00	1693686.13
30.00	769960.63	0.00	0.00	0.00	1568925.63
35.00	839931.56	0.00	0.00	0.00	1507813.63
40.00	898703.13	0.00	0.00	0.00	1458015.88
45.00	948068.06	0.00	0.00	0.00	1417476.38
50.00	989532.00	0.00	0.00	0.00	1384930.63
55.00	1024359.50	0.00	0.00	0.00	1358800.00
60.00	1053612.63	0.00	0.00	0.00	1288208.38
65.00	1078183.38	0.00	0.00	0.00	1272111.13
70.00	1098821.50	0.00	0.00	0.00	1260260.13
75.00	1116156.50	0.00	0.00	0.00	1251715.50
80.00	1130717.13	0.00	0.00	0.00	1245824.63
85.00	1142947.25	0.00	0.00	0.00	1242389.00
90.00	1153219.63	0.00	0.00	0.00	1190907.13
95.00	1161848.00	0.00	0.00	0.00	1190680.75
100.00	1169095.38	0.00	0.00	0.00	1192192.88
105.00	1175182.88	0.00	0.00	0.00	1194962.25
110.00	1180295.88	0.00	0.00	0.00	1198692.88
115.00	1184590.63	0.00	0.00	0.00	1203225.00
120.00	1188198.00	0.00	0.00	0.00	1158267.75
125.00	1191228.00	0.00	0.00	0.00	1163669.38
130.00	1193773.00	0.00	0.00	0.00	1169959.00
135.00	1195910.38	0.00	0.00	0.00	1176595.13
140.00	1197705.88	0.00	0.00	0.00	1183622.63
145.00	1199214.13	0.00	0.00	0.00	1190875.38
150.00	1202522.88	0.00	0.00	0.00	1148264.88
155.00	1206490.88	0.00	0.00	0.00	1156732.25
160.00	1209607.00	0.00	0.00	0.00	1166020.50
165.00	1212224.50	0.00	0.00	0.00	1175813.13
170.00	1214422.88	0.00	0.00	0.00	1185941.13
175.00	1216269.63	0.00	0.00	0.00	1196494.75
180.00	1217820.50	0.00	0.00	0.00	1157115.13
185.00	1219123.38	0.00	0.00	0.00	1168003.75
190.00	1220217.63	0.00	0.00	0.00	1179261.50
195.00	1221136.75	0.00	0.00	0.00	1190667.00
200.00	1221908.75	0.00	0.00	0.00	1202240.63

FIGURE B.22. Output File REGMAS.OUT

```

*****
*
*                               SHIMS.OUT FROM MASBAL
*
* Title: MASBAL TEST CASE
*
* User:  PAUL REIMUS
*
* Date:   5-MAY-1987
*
* Time:  15:56:06
*
*****

```

FEED SHIM

DATA FROM FSHIM.DAT

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	200.000	210.000	210.000
END	0	0.000	0.000	0.000

STARTING TIME FOR FEED SHIM = 50.0008
METHOD OF ANALYSIS OF COMPOSITION = 1

CALCULATED COMPOSITION OF SHIM

CONSTITUENT	G OXIDE/L	NSAM	NANL
SI02	213.562	1	1
B2O3	0.000	0	0
NA2O	0.000	0	0
FE2O3	0.000	0	0
K2O	0.000	0	0
CS2O	0.000	0	0
SRO	0.000	0	0
NIO	0.000	0	0
ZNO	0.000	0	0
OTHER	0.000	0	0

STOP TIME FOR FEED SHIM = 50.0031

COMPOSITION IN FEED TANK AFTER SHIM

CONSTITUENT	G OXIDE/L
SI02	123.943
B2O3	67.247
NA2O	36.070
FE2O3	27.449
K2O	28.692
CS2O	1.653
SRO	1.747
NIO	14.086

FIGURE B.23. Output File SHIMS.OUT

ZNO 13.771
OTHER 34.932

MELTER SHIM

DATA FROM MSHIM.DAT

CONSTITUENT	N	ANALYSIS 1	ANALYSIS 2	ANALYSIS 3
SI02	1	200.000	210.000	210.000
END	0	0.000	0.000	0.000

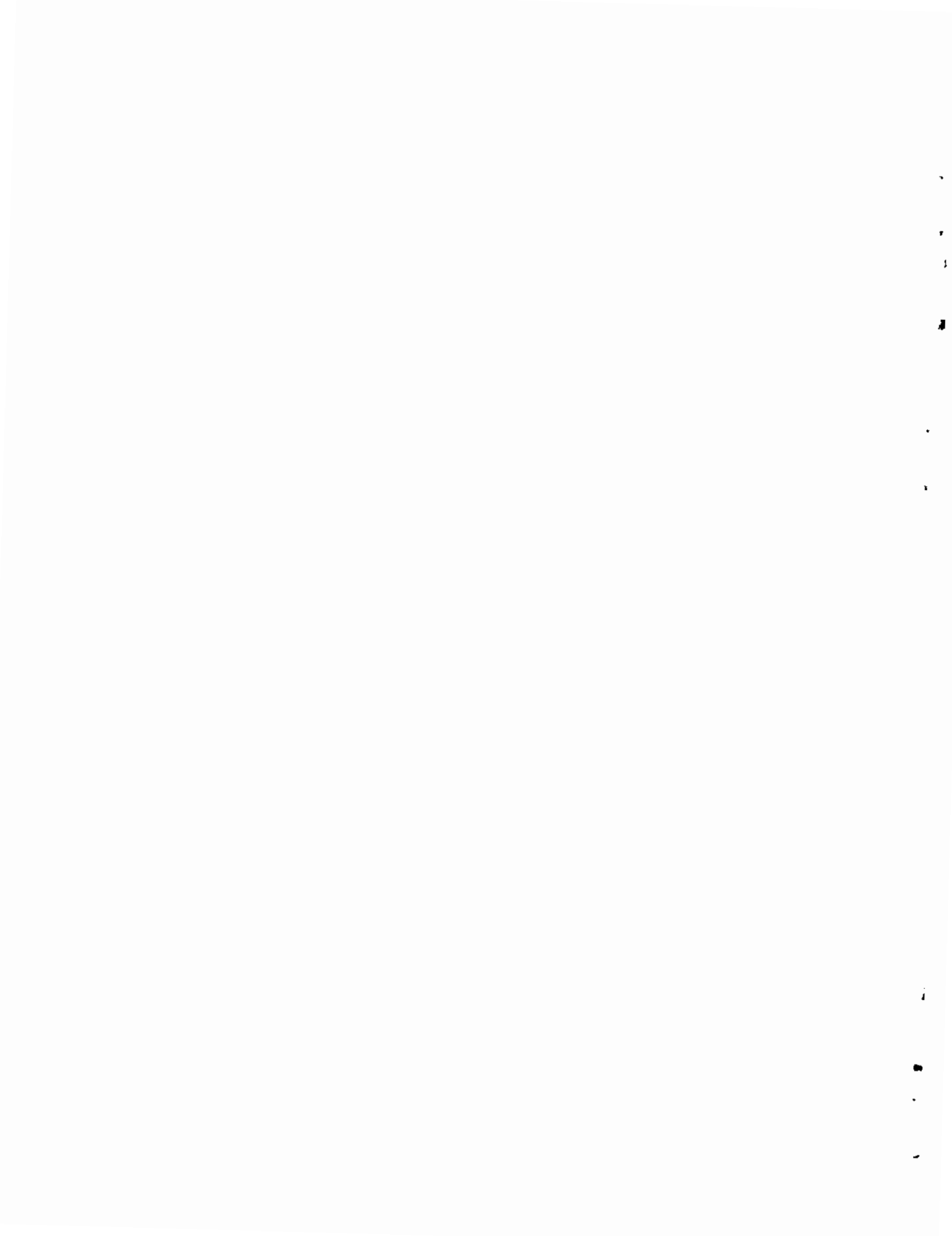
STARTING TIME FOR MELTER SHIM = 149.9990
METHOD OF ANALYSIS OF COMPOSITION = 1

CALCULATED COMPOSITION OF SHIM

CONSTITUENT	G OXIDE/L	NSAMM	NANLM
SI02	171.575	1	1
B2O3	0.000	0	0
NA2O	0.000	0	0
FE2O3	0.000	0	0
K2O	0.000	0	0
CS2O	0.000	0	0
SRO	0.000	0	0
NIO	0.000	0	0
ZNO	0.000	0	0
OTHER	0.000	0	0

STOP TIME FOR MELTER SHIM = 150.0014

FIGURE B.23. (contd)



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