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TOPAZ - The Transient One-Dimensional Pipe Flow Analyzer: User's Manual

W. S. Winters

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TOPAZ - The Transient One-Dimensional Pipe Flow Analyzer:
User's Manual

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Manuscript Completed March 14, 1985

ABSTRACT

TOPAZ is a "user friendly" computer code for modeling the one-dimensional-transient physics of multi-species gas transfer in arbitrary arrangements of pipes, valves, vessels, and flow branches. This document serves as a user's manual for the code, and should provide potential users with enough information to take advantage of many of the code's capabilities. Details regarding equations and numerics, example problems, applications, and modeling assumptions will be discussed in companion documents.

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FORWARD

This report serves as a user's manual for the computer code, TOPAZ. TOPAZ is an acronym for (T)ransient-(O)ne-dimensional (P)ipe flow (A)naly(Z)er. The code was developed at Sandia Laboratories, Livermore, CA, but it can be transported to other institutions, without great difficulty, by altering the machine dependent coding.

The text in Sections I thru VI of this report is a replication of the online public text file "TOPAZAID". The text in the file TOPAZAID is "dynamic" in the sense that it is updated each time changes are made to TOPAZ. Hence, users can be constantly kept abreast of new developments in TOPAZ by viewing the file TOPAZAID. Sections I thru VI of this report represent the status of the code at the time of this publication.

Although Sections I thru VI provide potential users with enough information to utilize most of TOPAZ's capabilities, this report contains additional information in the form of three appendices. Appendix A contains a more complete discussion of the comprehensive example (EXAMPLE 3) given in Section III. TOPAZ output listings from the example are presented and discussed and calculational results are shown in graphical form. This information is difficult to present in a computer generated document having an 80 column width. Appendix B contains a discussion of how to incorporate moving control volume boundaries (sliding pistons) into gas transfer calculations. In the last appendix, Appendix C, additional modeling considerations are discussed. The information in Appendices B and C was not included in the TOPAZAID file in order to keep that document concise.

Because this report is a user's manual, only a superficial discussion of the modeling physics, modeling assumptions, and numerical techniques is presented. Users interested in more detail are invited to consult the references listed in Section VI or to contact the author directly. More TOPAZ documentation will soon be available to outline additional examples and the code's equations and numerics.

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I. INTRODUCTION

TOPAZ is a computer code for modeling the one-dimensional-transient physics of multi-species gas transfer in arbitrary arrangements of pipes, valves, vessels, and flow branches. The name "TOPAZ" is an acronym for (T)ransient (O)ne-dimensional (P)ipe flow (A)naly(Z)er.

This computer generated document serves as a "dynamic" users manual for TOPAZ. Since TOPAZ is an evolving code with new features being added on a continuing basis, a means of notifying potential users of TOPAZ improvements had to be developed. It is intended that this dynamic document serve as an up to date "snap shot" of TOPAZ user instructions and code capabilities. As improvements and additions are made to the code, this document will be updated. Users can access the most recent version of this document viewing, copying, or printing the public file TOPAZAID.

In the course of reading this document, it is hoped that potential users will become aware of the available options for modeling the flow of compressible gas mixtures through piping networks. These options include equation of state mixture models, transport property models, heat transfer models, and pressure loss models. The current state of the code is believed to be appropriate for modeling a large class of gas transfer problems of interest to Sandia, however, TOPAZ development is by no means limited to the options outlined here. TOPAZ has been written in a modular fashion which facilitates improvement of existing models and the addition of new models. Users interested in expanding the code's capabilities to suit a particular need are encouraged to consult with the author.

TOPAZ provides a means of analyzing complex gas transfer systems with a relatively superficial knowledge of compressible flow, finite differences, and implicit numerical methods. In the interest of conciseness such details will not be discussed in this computer generated document. For those users interested in the more detailed aspects of TOPAZ modeling, References (1) through (6) are available in Section VI. These references provide background information on equations and numerics, and modeling assumptions. More complete information will be published shortly. This information will provide users with additional TOPAZ examples, real applications, and code validation.

TOPAZ currently resides on the CRAY/CTSS computers at Sandia Livermore. In order to use TOPAZ, users must create a CTSS text input file (default name "ifile") before executing the code. During execution TOPAZ creates (or overwrites) two additional CTSS text files, one for the output listing (default name "ofile") and one for plot post processing (default name "pfile"). The complete CTSS command for TOPAZ execution is "topaz i=ifile,o=ofile,p=pfile". Other file names may be used in place of the default names, for example: "topaz i=cat,o=dog,p=moose".

This document will discuss how to construct the TOPAZ input file and provide potential TOPAZ users with enough information to produce comprehensive models for analyzing complex gas transfer systems and related compressible flow problems.

The steps that TOPAZ takes in producing compressible flow calculations can be summarized as follows:

1. The user's input data is read one line at a time from the input file. The code checks for syntax errors after reading in each line.
2. When the entire input file is read, the code analyzes the input data for completeness and consistency.
3. The code employs dynamic dimensioning to expand memory to accomodate the size of the user's problem.
5. The code generates the TOPAZ computational mesh for producing one-dimensional-transient finite difference calculations along all flow paths.
6. Appropriate mesh generation tables and initial conditions are printed into the output file.
7. The code employs the implicit differential/algebraic solver, DASSL (4) to perform integrations in time.
8. Computational results are printed into the output file and plot post processing file at user specified frequencies.

Before the user can construct the TOPAZ input file or read the TOPAZ output files, some consideration must be given to the units which are assumed for the numerical data. All numerical input data and printed output is assumed to conform to the International System of Units (SI), the system currently endorsed by the United States Department of Commerce, National Bureau of Standards. These units are summarized as follows:

Length	=meters (m)
Time	=seconds (s)
Mass	=kilograms (kg)
Force	=Newton ($N=kg\cdot m/s^2$)
Pressure	=Pascal ($Pa=N/m^2$)
Temperature	=Kelvin (K)
Energy	=Joule ($J=N\cdot m$)
Mole density	= $kg\cdot mol/m^3$

II. CONSTRUCTING THE TOPAZ INPUT FILE

The input file must contain the user's mesh generation information (network geometry), initial conditions, instructions for execution, and instructions for printing the output.

Users have a high degree of flexibility in creating the input file. Each line of the input file need only have the form,

DIRECTIVE = NUMERICAL DATA

The "directive" is a string of keyboard characters (letters, numbers, blanks, and/or any other keyboard character except the "=" sign). The only rule for communicating an input directive to TOPAZ is that the first four non blank characters must be uppercase letters A thru Z. These four characters have a specific meaning to the TOPAZ user interface. The remaining characters in the directive are totally arbitrary and may be used to imbed special notes or messages which are significant to the user.

The "=" sign is used to separate the directive from the corresponding piece of numerical data. There must be one and only one "=" sign per line of data.

The numerical data which appears to the right of the "=" sign usually consists of a single number. This number may be in any format, in any column, and with any number of intervening blanks providing the entire data line does not exceed 80 characters.

As an example of the TOPAZ "directive = numerical data" input structure consider the following four input data lines, all of which would be interpreted in precisely the same way:

```
PIPE=26
P   I   PE                      =          2          6.
PIPE (downstream of supply)=+26.0000000
PIPE                               =+.26e+02
```

There are two variations on the "directive=numerical data" input structure. These have to do with inserting comments (NOTE directive) and specifying which variables to print during minor edits (EFLAG directive). These exceptions are summarized as follows:

1. When the first four non blank characters in a line are the letters "NOTE", the line is not interpreted as a data line but rather as a comment. The user may type any keyboard characters after the "E" providing the entire line does not exceed 80 characters.

2. The EFLAG directive (explained later) is the only data line which takes the form: "EFLAG=number,number" In this case two pieces of numerical data are associated with the directive. This data can appear in any column, in any format, and with any number of intervening blanks providing the two numbers are separated by a "comma" and the entire data line does not exceed 80 characters.

A few words are appropriate regarding how TOPAZ models compressible flow problems. Flow models of arbitrary piping networks are formed by linking together two types of fluid elements, the continuity-energy (CE) element and the momentum (M) element. The only acceptable method for modeling a flow path is the alternating arrangement represented by the string CE-M-CE-M-CE-....etc. In subdividing the flow path it is useful to think of the CE elements as being physical volumes and M elements as being the interface between adjacent CEs. Since M elements act as CE boundaries they possess no physical volume. Hence if a constant diameter pipe is subdivided into 10 equal CEs the volume of gas residing in each CE at any instant of time is the one tenth the volume of the pipe.

By representing the flow path with alternating CEs and Ms, the user has in effect generated an upwind finite difference mesh which can be used to numerically solve the one-dimensional-transient compressible flow conservation equations along the flow path. This process and additional modeling assumptions are discussed in Reference (1).

EXAMPLE 1. Suggest an arrangement of CEs and Ms which could be used to model the flow of a gas from a high pressure reservoir to a low pressure receiver vessel via a long constant diameter pipe.

In TOPAZ, a single CE may be used for each of the major vessels (reservoir and receiver). Using a single CE element to model an entire vessel implies that all properties within the vessel are uniform in space. Hence at any instant of time within the vessel, the contents exist at a uniform pressure, temperature, composition, etc.

Flows in pipes usually require a resolution of the axial spacial dependence. Hence, it will be more accurate to model the pipe flow using a string of alternating CE and M elements rather than with a single CE element as is frequently done for vessels. In this example, the pipe will be simulated with a string alternating CEs and Ms beginning and ending with a CE.

In order to avoid direct contact of two adjacent CEs, an M element will have to be used to join the reservoir to the upstream end of the pipe. Similarly a second M element will be required to join the downstream end of the pipe to the receiver.

In our example, for the case where the pipe is modeled using 6 CEs the arrangement of CEs and Ms takes the following form:

CE - M - CE-M-CE-M-CE-M-CE-M-CE-M-CE - M - CE

R
E
S
E
R
V
O
I
R

P
I
P
E

R
E
C
E
I
V
E
R

For a long pipe, using 6 CEs could represent a relatively coarse and potentially inaccurate finite difference mesh. Accuracy may require as many as 20 or more CEs. It quickly becomes apparent that direct use of CEs and Ms to describe the piping network could lead to an extremely tedious input process since the user would be required to supply a whole set of data for each CE or M (e.g. diameter, length, initial conditions, etc.)

In order to avoid the direct use of CEs and Ms to describe the piping network, the TOPAZ user interface has been designed to interpret major "component" directives rather than directives for individual CEs and Ms. Currently TOPAZ recognizes 3 component directives to describe collections of CE and M elements. These component directives are described as follows:

CHAMBER - A CHAMBER is a CE designed to represent an entire vessel, branch volume, or short single control volume pipe. The shortest typed form for this directive is the four letter string "CHAM".

PIPE - A pipe is a chain of alternating CEs and Ms beginning and terminating with a CE. For example: CE-M-CE-.....-M-CE-M-CE. Such an arrangement could be used to simulate flow through a constant diameter pipe or tube, or even a single long vessel in those situations where it is important to resolve the one-dimensional-transient physics within the vessel. The shortest typed form for this directive is the four letter string "PIPE".

JOINT - A JOINT is an M which can be used to link CHAMBERS to CHAMBERS, PIPES to PIPES, or CHAMBERS to PIPES. JOINTS may act as orifices, ID changes, or valves which open and/or close during the flow simulation. The shortest typed form for this directive is the four letter string "JOIN".

A fourth major component directive, which will be discussed in more detail in future documentation, is designed to account for the motion CHAMBER walls. Such motion is typically encountered in systems having sliding pistons, rolling bladders, etc. This fourth component is called a PISTON and is described as follows:

PISTON - A PISTON is a physical boundary isolating two adjacent CHAMBERS. The PISTON may or may not have an associated physical mass (inertia) and may or may not be constrained by breakaway, spring, viscous friction, and/or coulomb friction forces. The shortest typed form for this directive is the four letter string "PIST".

The linking together of CHAMBERS, PIPEs, JOINTs, and PISTONs to form a the TOPAZ model for a piping network is arbitrary providing one follows these simple rules:

1. Never connect CHAMBERS and PIPEs without a JOINT in between.
2. JOINTs must connect 2 and only 2 CHAMBERS and/or PIPEs.
3. A maximum of 6 JOINTs can be connected to any 1 CHAMBER.
4. A maximum of 1 JOINT can be connected to a PIPE end.
5. A CHAMBER may have no more than one moving boundary (PISTON).
6. A PISTON must have one and only one CHAMBER on its upstream (high pressure) side and one and only one CHAMBER on its downstream (low pressure) side.

Components are distinguished from each other in the input file by assigning numbers to each component. Three rules must be followed in numbering major components:

1. Component numbering is sequential beginning with the number "1".
2. All PIPEs must be numbered last.
3. CHAMBERS, JOINTs, and PISTONs may be numbered in any order providing rules 1 and 2 are not violated.

The remaining examples and discussion in this document will focus on the the most frequently used TOPAZ components, namely CHAMBERS, PIPEs, and JOINTs.

EXAMPLE 2. Suggest an arrangement of CHAMBERS, PIPEs and JOINTs which could be used to mesh the problem of EXAMPLE 1.

The linking together and numbering of CHAMBERS, PIPEs, and JOINTs for this problem can be represented as follows:

COMPONENT ARRANGEMENT: CHAMBER-JOINT-PIPE-JOINT-CHAMBER
COMPONENT NUMBERING: 1 3 5 4 2

The first four uppercase letters for these components represent TOPAZ recognized directives. Hence one could communicate the component numbering to TOPAZ in the input file as:

```
CHAM=1
JOIN=3
PIPE=5
JOIN=4
CHAM=2
```

These data lines specify the component numbering only. No information has been communicated to indicate the relationship of these components to each another in the piping network (more about that later). Input data lines for alternative numbering scheme could take the form:

```
CHAMBER (reservoir)=1
JOINT (valve)=2
J O I N              =      3.e+00
CHAMBER (receiver)=4.000000
PIPE (TRANSFER TUBING)= 5
```

Note that this is still an acceptable numbering scheme since the PIPE component was numbered last. The ordering of the directives as well as the numbering of CHAMBERS and JOINTs (and PISTONS) is arbitrary providing the numbering is sequential beginning with the number 1. These data lines again illustrate the nearly free-form flexibility in communicating directives in the input file.

The CHAMBER, PIPE, JOINT and PISTON component directives represent four of the seven TOPAZ "major directives". The remaining three major directives are described below:

- REGION - This directive is used in specifying initial conditions (i.e. initial gas mixture composition, temperature, and pressure or molar density). All components are assigned to specific "REGIONS" in the input file. The method used in making this assignment is discussed later. The shortest typed form for this directive is the four letter string "REGI".
- EXECUTION - This directive is used to specify how the problem is to be executed, the length of the execution, the frequency for printing output, etc. The shortest typed form for this directive is the four letter string "EXEC".
- EDIT - This directive is used to specify which variables to print during "minor edits". Minor edits and the use of the EDIT directive will be discussed later. The shortest typed form for this directive is the four letter string "EDIT".

Thus far, only the seven TOPAZ major directives have been discussed. Associated with each of these major directives is a family of "minor directives" which serve to further define or communicate information about the major directive. Minor directives appear on lines in the input file immediately following the associated major directive. When TOPAZ encounters a major directive in the input file it interprets each subsequent directive as a minor directive until a new major directive is encountered. As an example of how major and minor directives might appear in an input file, consider the following list which might be used to describe a particular pipe in a TOPAZ simulation:

```
PIPE=26
  DIAMETER=.001
  LENGTH=1.604
  NUMBER OF CE's=10
  HFLAG=1
  FFLAG=2
  FDATA=.01
  INITIAL CONDITIONS=2
```

In the example above the seven minor directives have been indented to distinguish them from the associated major directive "PIPE=26". This indenting improves the readability of the input file for the user but is not required.

The order in which the minor directives appear is arbitrary. If the user chooses, the minor directives could be reordered and the four letter abbreviations used for all directives, i.e.,

```
PIPE=26
INIT=2
FDAT=.01
FFLA=2
HFLA=1
NUMB=10
LENG=1.604
DIAM=.001
```

The precise meaning of the seven minor pipe directives (and all other minor directives) are outlined in Tables 1 through 7. Some minor directives will have defaults. When an appropriate default is available the user need not enter the minor directive in the input file. In general, the default directive values were selected to reflect situations most frequently encountered in modeling the flow of real gases through actual piping networks. For those directives which have no defaults available, the user must supply the directive in the input file. Failure to do so will terminate the processing of input data and produce an appropriate error message.

Much of the numerical input data associated with the major and minor directives are unitless. As mentioned previously, any data having physical units (e.g., time, length, volume, pressure, etc.) must be expressed in SI. In Tables 1 through 7 the units for such data are shown in parenthesis following each directive description.

Tables 1 through 7 represent a concise reference for TOPAZ modeling. Information on each and every major and minor directive is presented. Many of the directive descriptions may appear incomplete on first reading but it is hoped that the discussion in Section III will describe more fully the use of these directives in creating the TOPAZ input file.

Every effort has been made to "foolproof" the TOPAZ user interface and mesh generator. The code will not allow improper data, or physically unrealistic finite difference meshes to be generated. If the user inadvertently inputs erroneous data, a brief informative message will be printed into the output file and computations will terminate. Any users detecting improper or incomplete screening of their input data are encouraged to contact the author. User feedback is an important factor in further TOPAZ development and improvement.

Table 1. The CHAMBER Directive and Associated Minor Directives

DIRECTIVE	DESCRIPTION	DEFAULT
CHAM	Major directive which assigns a unique component number to a particular CHAMBER.	none
DIAM	CHAMBER diameter. (m)	none
VOLU	CHAMBER volume. The user may find it more convenient to substitute this directive in place of the DIAM directive. The code will then calculate the appropriate value of DIAM based on the input value for VOLU (and if appropriate LENG). Either DIAM or VOLU must be supplied for each CHAMBER. (m ³)	none
LENG	CHAMBER length. When LENG=0, the chamber is assumed to be spherical in shape with a diameter of DIAM. When a non zero value is used, the chamber takes on the shape of a cylinder having a length and diameter of LENG and DIAM respectively. (m)	0
HFLA	CHAMBER heat transfer coefficient flag used to model the heat exchange between the chamber walls and the resident gas mixture. HFLA=1 Adiabatic case, $h=0$. HFLA=2 Isothermal case, $h=\text{infinite}$. HFLA=3 Pipe flow forced convection, $h=f(\text{Re}, \text{Pr})$. HFLA=4 Vessel free convection, $h=f(\text{Ra})$.	4
GENE	Mass generation rate within CHAMBER. Mass is generated only for the time perion between GSTA and GSTO. (kg/s)	0.
GSTA	Time when mass generation (GENE) initiates. (s)	infinite
GSTO	Time when mass generation (GENE) terminates. (s)	0.
INIT	CHAMBER initial conditions flag used to identify the REGION number in which the CHAMBER resides.	none

Table 2. The PIPE Directive and Associated Minor Directives

DIRECTIVE	DESCRIPTION	DEFAULT
PIPE	Major directive which assigns a unique component number to a particular pipe.	none
DIAM	PIPE diameter. (m)	none
LENG	PIPE length. (m)	none
HFLA	PIPE heat transfer coefficient flag used to model the heat exchange between the pipe walls and the resident gas mixture. HFLA=1 Adiabatic case, $h=0$. HFLA=2 Isothermal case, $h=\text{infinite}$. HFLA=3 Pipe flow forced convection, $h=f(\text{Re}, \text{Pr})$.	3
FFLA	PIPE friction factor flag used to model pipe wall frictional effects on the flowing resident gas mixture. FFLA=1 User specified constant Darcy friction factor will be used, $f=\text{FDAT}$. FFLA=2 Moody friction factor model where Darcy friction factor is a function of the local Re and tube wall relative roughness, $f=f(\text{Re}, \text{FDAT})$.	2
FDAT	PIPE friction data. FDAT= User specified constant Darcy f (for FFLA=1). FDAT= User specified global pipe wall roughness ratio (roughness height/diameter) used in the Moody friction factor computation (for FFLA=2).	0.
NUMB	Number of CEs to be used in representing the PIPE.	none
INIT	PIPE initial conditions flag used to identify the REGION number in which the PIPE resides.	none

Table 3. The JOINT Directive and Associated minor directives

DIRECTIVE	DESCRIPTION	DEFAULT
JOIN	Major directive assigning component number to JOINT.	none
UPST	Flag identifying the number of the component (i.e. PIPE or CHAMBER) located upstream of the JOINT. The UPST and DOWN directives establish the sign convention for positive flow (upstream to downstream).	none
DOWN	Flag identifying the number of the component (i.e. PIPE or CHAMBER) located downstream of JOINT.	none
DIAM	Diameter of the JOINT flow path. When this directive is not used, the upstream or downstream component diameter will be assumed depending on which is the smallest (minimum). (m)	minimum
KFLA	JOINT form loss flag used to model flow losses. KFLA=1 User constants for forward/reverse flow. KFLA=2 User specified formula. Consult Author. KFLA=3 Approximates isentropic flow. (no losses)	1
FLOS	User specified form loss constant for forward flow (i.e. upstream to downstream). Used when KFLA=1.	0.
RLOS	User specified form loss constant for reverse flow (i.e. downstream to upstream). Used when KFLA=1.	0.
TOPE	Time at which JOINT opens. When this directive is used the JOINT becomes a valve having a time dependent flow area. The valve is closed at time=0 and starts to open at time=TOPE. (s)	infinite
DTOP	Time required to open a closed JOINT. The flow area increase is approximately linear with time. (s)	infinite
TCLO	Time at which JOINT closes. When this directive is used the JOINT becomes a valve having a time dependent flow area. The valve is open at time=0 and then begins to close at time=TCLO. If both the TOPE and TCLO directives are specified for a JOINT, it becomes a valve that is closed at time=0, starts to open at time=TOPE, and starts to close at time=TCLO. When both TOPE and TCLO are specified, TOPE+DTOP must be less than TCLO. (s)	infinite
DTCL	Time required to close an open JOINT. The flow area decrease is approximately linear with time. (s)	infinite

Table 4. The PISTON Directive and Associated Minor Directives.

DIRECTIVE	DESCRIPTION	DEFAULT
PIST	Major directive which assigns a unique component number to a particular PISTON.	none
UPST	Flag identifying the CHAMBER number located on the assumed high pressure side of the PISTON. The UPST and DOWN directives establish the sign convention for piston motion. Positive displacement and velocities imply PISTON movement from the upstream direction to the downstream direction.	none
DOWN	Flag identifying the CHAMBER number located on the assumed downstream side of the PISTON.	none
XMUP	The maximum allowable travel distance in the upstream direction, i.e. position of a mechanical stop. (m)	0.
XMDN	The maximum allowable travel distance in the downstream direction, i.e. position of a mechanical stop. (m)	0.
FBRE	Breakaway force, i.e. force which must be overcome prior to the initial piston movement. (N)	0.
XKZE	The value of x (PISTON displacement coordinate) where the PISTON spring force is zero. (m)	0.
MASS	PISTON mass. (kg)	0.
CVIS	PISTON viscous damping factor. (N-s/m)	0.
KSPR	PISTON spring constant. (N/m)	0.
AREA	PISTON cross-sectional area. (m ²)	0.
AFAC	PISTON cross-sectional area multiplier.	1.
FCOU	PISTON coulomb friction force. (N)	0.
FORC	Applied constant force. (N)	0.
FSTA	Time when constant force (FORC) is applied. (s)	infinite
FSTO	Time when constant force (FORC) is removed. (s)	0.

Note: TOPAZ assigns 0 velocity and 0 position for PISTON initial conditions.

Table 5. The REGION Directive and Associated Minor Directives.

DIRECTIVE	DESCRIPTION	DEFAULT
REGI	Major directive which assigns a unique number to a particular REGION.	none
TEMP	Initial temperature for gas occupying the REGION. (K)	295.
TWAL	Wall temperature for all components in the REGION. The wall temperature remains constant with time. (K)	295.
MIXT	Flag that identifies which equation of state and transport properties will be used in the calculations. Currently the following options are available: MIXT=1 Ideal gas (Dalton) model for the five species mixture of H ₂ , O ₂ , T ₂ , HE ₃ , HE ₄ . Constant ambient temperature transport properties. MIXT=2 Abel-Nobel real gas model for the five species mixture of H ₂ , O ₂ , T ₂ , HE ₃ , HE ₄ . Variable transport properties. MIXT=3 Clark-Ashurst model for the five species mixture of H ₂ , O ₂ , T ₂ , HE ₃ , HE ₄ . Variable transport properties. This model is useful when using TOPAZ to produce "fillup" calculations but is not recommended for time integrations, i.e. transient modeling. MIXT=4 Abel-Nobel real gas model for the five species mixture of H ₂ , O ₂ , T ₂ , HE ₃ , HE ₄ . Constant ambient temperature transport properties. This is a good choice for "debugging" runs.	2
PRES	Pressure of gas mixture occupying the REGION. User may choose to specify the mixture molar density instead of the pressure but one of these two minor directives must be present for all REGIONS. If both (or neither) are present, the processing of input data will terminate with an appropriate message. (Pa)	none
DENS	Molar density of all gas occupying the REGION. The user may choose to specify the pressure instead of the molar density but one of these two minor directives must be present for all REGIONS. If both (or neither) are present, processing of input data will terminate with an appropriate message. (kg-mol/m ³)	none
GAS1	Initial mole fraction for first species of gas in mixture (e.g. mole fraction of H ₂ when MIXT=1,2,3, or 4). If this directive is not present the first species will not be included in the computations. The GAS1 should not appear in the input file when it is known that it is impossible for species 1 to ever occupy any portion of the REGION. Not including a gas species in the calculations results in a substantial decrease in computational time. If the REGION is initially void of species 1 but it is physically possible for this species to occupy any portion of the REGION at a later time, then the correct form of this directive is GAS1=.0	none
GAS2	Initial mole fraction for the second species of gas in the gas mixture. The explanation for the GAS1 directive also applies to this directive.	none
GAS3	Initial mole fraction for the third species of gas in the gas mixture. The explanation for the GAS1 directive also applies to this directive.	none
GAS4	Initial mole fraction for the forth species of gas in the gas mixture. The explanation for the GAS1 directive also applies to this directive.	none
GAS5	Initial mole fraction for the fifth species of gas in the gas mixture. The explanation for the GAS1 directive also applies to this directive.	none

Table 6. The EXECUTION Directive and Associated Minor Directives.

DIRECTIVE	DESCRIPTION	DEFAULT
EXEC	Major directive which determines the extent of TOPAZ execution. EXEC=0 Read and process data, generate mesh, print mesh generation tables if appropriate, print initial conditions, then terminate without performing time integrations. EXEC=1 Same as EXEC=0 except the time integrations are performed.	none
LIST	Directive which permits printing of special listings in addition to those generated in output from time integrations. LIST=0 No additional listings LIST=1 User/TOPAZ mesh generation information LIST=2 Input Dump+User/TOPAZ mesh info LIST=3 TOPAZ Dump+Input Dump+User/TOPAZ Mesh info Options 2 and 3 are not useful to most users.	1
TSTO	Time when time integrations will stop. (s)	0.
DTMA	Time frequency for producing Major Edits. Major Edits are printouts of variables at each and every CE, M and PISTON element. Pressures are printed at each CE, velocities are printed at each M and piston position is printed at each PISTON element. DTMA should be an integer multiple of DTMI. (s)	1.E30
DTMI	Time frequency for producing Minor Edits. Minor Edits are printouts of up to six variables, the identity of which is determined by the EDIT directives. See Table 6 for a discussion of Minor Edits. (s)	1.E30
ATOL	Absolute integrator error tolerance. See Reference (4).	1.E-3
RTOL	Relative integrator error tolerance. See Reference (4).	1.E-3
DAMP	Finite difference artificial viscosity factor, useful in resolving steep shocks. See Reference (6).	0.

Table 7. The EDIT Directive and Associated Minor directives.

DIRECTIVE	DESCRIPTION	DEFAULT
EDIT	Major directive identifying the number of variables to be included in the minor edits. Minor edit variables are printed onto the output file and onto the plot post processing file.	0
EFLA	EFLA directives must be supplied if EDIT is non zero. The EFLA directive takes the form "EFLA=i,j" where i and j are free format numbers which will be truncated to integers. There must be one EFLA directive for each variable printed during minor edits. The i entry identifies the element (CE, M, or PISTON) to be edited. In some cases the User/TOPAZ mesh generation will be required to determine the numbering of CEs and Ms. This is particularly true when EDIT elements are CEs and Ms which lie in PIPES. For JOINTs, CHAMBERs, and PISTONs the component and the element numbers are identical. For CE and M elements the j entry identifies which of 15 element variables will be printed during the minor edit: j=1 Temperature, edit symbol T j=2 Pressure, edit symbol P j=3 Internal energy per unit mass, edit symbol U j=4 Mass density, edit symbol R j=5 Mass of species 1, edit symbol M1 j=6 Mass of species 2, edit symbol M2 j=7 Mass of species 3, edit symbol M3 j=8 Mass of species 4, edit symbol M4 j=9 Mass of species 5, edit symbol M5 j=10 Total mass, edit symbol M j=11 Mass flow rate, edit symbol W j=12 Velocity, edit symbol V j=13 Volume, edit symbol VL j=14 Sonic Velocity, edit symbol VS j=15 Mach number, edit symbol MA For PISTON elements (or components) the j entry identifies which of three element variables will be printed during the minor edit: j=1 Piston position, edit symbol X j=2 Piston velocity, edit symbol V j=2 Piston kinetic energy, edit symbol KE	none

III. EXAMPLE INPUT FILE

The technique for constructing the TOPAZ input file can now be illustrated using the simple reservoir/receiver problem introduced in EXAMPLE 1.

EXAMPLE 3. Write the TOPAZ input file to simulate the transfer of a gas mixture from a high pressure spherical reservoir (diameter of .06 meters) to a low pressure cylindrical receiver (diameter of .2 meters and length of .4 meters) through a constant diameter pipe (diameter of .003 meters and length of 1.0 meters). Assume that a valve located between the reservoir and the pipe opens at time zero allowing gas to flow, then closes .25 seconds later causing the flow to stop. The time required to open or close the valve is .005 seconds. Initially the reservoir contains 1 gram of hydrogen (H_2) and 1 gram of helium (He_4). The pipe and receiver contain pure hydrogen at $6.8947E+3$ Pa (1 psi). The initial temperature throughout the network is 295 degrees K. The interior walls of the pipe are known to have a relative roughness ratio of .001. Assume the expansion into the receiver is isothermal but use appropriate heat transfer modeling for the reservoir and pipe. It is desired to calculate the time history of the following quantities for .5 seconds:

1. Reservoir pressure
2. Reservoir temperature
3. Receiver pressure
4. Mass flow rate through the valve
5. Mass of H_2 in the receiver
6. Mass of HE_4 in the receiver

This example illustrates the two basic ways for specifying initial conditions. In the reservoir, the temperature and hydrogen/helium masses are known but not the pressure. In the receiver and pipe, the temperature and pressure are known but not the mass of pure hydrogen. In most TOPAZ gas transfer simulations, initially closed valves provide the most logical boundaries for defining REGIONS. In this case the reservoir can be assigned to REGION 1 and the pipe and receiver to REGION 2. In order to write the minor directives for REGION 1, it is first necessary to compute the mixture molar density and the component mole fractions. This is a straightforward calculation involving the masses of the components, their molecular weights and the volume occupied by the gas mixture. For REGION 1 the mixture molar density is 6.595 kg-mol/cubic meter and the mole fractions of hydrogen and helium are .665 and .335 respectively. The minor directives for REGION 2 can be written immediately since the pressure is known and the mole fractions of hydrogen and helium are known to be 1.0 and 0. respectively.

The following steps are recommended for component numbering in this or any other problem:

1. Draw a simple sketch representing the network. Use large circles to represent CHAMBERS, solid dots to represent JOINTs, and solid lines to represent PIPEs. If appropriate include PISTONs.
2. Number the CHAMBERS (circles) and JOINTs (solid dots) consecutively in any order beginning with the number 1. If PISTONs are being modeled, include them in the numbering.
3. Number the remaining PIPEs (solid lines).
4. Assign arbitrary flow directions for all flow paths between CHAMBERS by drawing arrows to indicate the direction of flow. Use a single arrow through any piston to define the assumed direction for positive displacement.
5. The indicated flow directions should then be used to assign the UPSTREAM and DOWNSTREAM flags for all JOINTs. Assume the arrows point from upstream to downstream. When values for flow rate and velocity are printed into the output file, the sign will reflect the user's assumed direction of flow, positive implies flow from upstream to downstream, negative implies downstream to upstream.

The complete TOPAZ input file for EXAMPLE 3 is listed in Table 8. Each directive is explained through the use of imbedded comments and longer than necessary directive names. This file also contains a number of directives which are available as defaults. It is not necessary for these directives to appear in the input file but they are included here for illustrative purposes. This same input file could have been generated with a minimum of typing by dispensing with comments, using 4 letter directives, and making full use of the default directives. Table 9 contains this shorter form for the TOPAZ input file. Each input file will produce precisely the same TOPAZ calculations.

Table 8. TOPAZ Input File for EXAMPLE 3 - Long Version

NOTE: The following list of major and minor directives illustrates
 NOTE: how to construct a TOPAZ input file for Example 3. Minor
 NOTE: directives are indented. SI units are assumed. Comments
 NOTE: are imbedded in parenthesis.

CHAMBER (REPRESENTS RESERVOIR)=1
 DIAMETER=.06
 HFLAG (FOR VESSEL HEAT TRANSFER)=4
 INITIAL CONDITIONS (THE RESERVOIR LIES IN REGION 1)=1
 CHAMBER (RECEIVER)=2
 DIAMETER=.2
 LENGTH (LENGTH REQUIRED TO SPECIFY CYLINDRICAL CHAMBER)=.4
 HFLAG (FOR AN ISOTHERMAL VESSEL)=2
 INITIAL CONDITIONS (THE RECEIVER LIES IN REGION 2)=2
 JOINT (REPRESENTS THE UPSTREAM VALVE)=3
 UPSTREAM COMPONENT=1
 DOWNSTREAM COMPONENT=5
 TOPEN (TIME WHEN VALVE OPENS)=0.
 DTOPEN (TIME REQUIRED TO OPEN)=.005
 TCLOSE (TIME WHEN VALVE IS CLOSED)=.25
 DTCLOSE (TIME REQUIRED TO CLOSE)=.005
 JOINT (REPRESENTS THE CONNECTION BETWEEN THE PIPE AND THE RESERVOIR)=4
 UPSTREAM COMPONENT=5
 DOWNSTREAM COMPONENT=2
 PIPE (REPRESENTS THE INTERCONNECTING PIPE)=5
 LENGTH=1.
 DIAMETER=.003
 NUMBER OF CHAMBERS (i.e., NUMBER OF CES)=20
 HFLAG (DEFAULT PIPE HEAT TRANSFER CORRELATION)=3
 FFLAG (DEFAULT MOODY FRICTION FACTOR CORRELATION)=2
 FOATA (RELATIVE INTERIOR TUBE WALL ROUGHNESS)=.001
 INITIAL CONDITIONS (THE PIPE LIES IN REGION 2)=2
 REGION (INITIAL CONDITIONS FOR GAS IN RESERVOIR)=1
 DENSITY (MOLAR DENSITY OF GAS MIXTURE)=6.595
 TEMPERATURE=295.
 TWALL (WALL TEMPERATURE)=295.
 GAS1 (MOLE FRACTION OF HYDROGEN PRESENT)=.665
 GAS5 (MOLE FRACTION OF HELIUM PRESENT)=.335
 MIXTURE FLAG (DEFAULT ABEL-NOBEL REAL GAS MIX OF H2,D2,T2,HE3,HE4)=2
 REGION (INITIAL CONDITIONS FOR GAS IN RECEIVER AND PIPING)=2
 PRESSURE OF GAS=6.8947E+3
 TEMPERATURE OF GAS=295.
 TWALL (WALL TEMPERATURE)=295.
 GAS1 (MOLE FRACTION OF HYDROGEN PRESENT)=1.
 GAS5 (MOLE FRACTION OF HELIUM PRESENT)=0.
 MIXTURE FLAG (DEFAULT ABEL-NOBEL REAL GAS MIX OF H2,D2,T2,HE3,HE4)=2
 EXECUTION=1
 LIST OPTION (PRODUCE USER TOPAZ MESH GENERATION TABLE)=1
 TSTOP (STOP CALCULATIONS WHEN TIME REACHES .5 SECONDS)=.5
 DTMAJOR (MAJOR EDIT FREQUENCY, i.e., ALL VALUES PRINTED)=.1
 DTMINOR (MINOR EDIT FREQUENCY, i.e., MINOR EDIT VARIABLES PRINTED)=.01
 EDIT (NUMBER OF MINOR EDIT VARIABLES)=6
 EFLAG (PRINT RESERVOIR PRESSURE)=1,2
 EFLAG (PRINT RESERVOIR TEMPERATURE)=1,1
 EFLAG (PRINT RECEIVER PRESSURE)=2,2
 EFLAG (PRINT MASS FLOW RATE AT JOINT 3)=3,11
 EFLAG (PRINT MASS OF HYDROGEN IN THE RECEIVER)=2,5
 EFLAG (PRINT MASS OF HELIUM IN THE RECEIVER)=2,9

Table 9. TOPAZ Input File for EXAMPLE 3 - Short Version

CHAM=1
DIAM=.06
INIT=1
CHAM=2
DIAM=.2
LENG=.4
HFLA=2
INIT=2
JOIN=3
UPST=1
DOWN=5
TOPE=0.
DTOP=.005
TCLO=.3
DTCL=.005
JOIN=4
UPST=5
DOWN=2
PIPE=5
DIAM=.003
LENG=1.
NUMB=20
FDAT=.001
INIT=2
REGI=1
DENS=6.595
GAS1=.665
GAS5=.335
REGI=2
PRES=6.8947E3
GAS1=1.
GAS5=0.
EXEC=1
TSTO=.5
DTMA=.1
DTMI=.01
EDIT=6
EFLAG=1,2
EFLAG=1,1
EFLAG=2,2
EFLAG=3,11
EFLAG=2,5
EFLAG=2,9

The output file generated by TOPAZ for this example problem is presented and discussed in Reference (5). Also presented is the time history for the six minor edit variables in plotted form.

IV. TOPAZ OUTPUT AND PLOT FILES

The TOPAZ output file (default name "ofile") contains the following information:

1. A line by line echo of the users input file
2. The requested special listings (e.g. User TOPAZ mesh table, etc.)
3. Major edits with appropriate labeling
4. Minor edits with appropriate labeling
5. Messages indicating location(s) and times when flow chokes/unchokes
6. Messages relating to piston motions
7. Integration error messages (Heaven Forbid!)

In addition to the output file, TOPAZ also produces a plot post process file (default name "pfile"). This file contains unlabeled columns of numbers in 7E13.4 format. Time is printed in the first column and the requested minor edit variables are printed in the remaining columns. The frequency for printing to the plot file is identical to the minor edit print frequency DTMINOR. The order of variables in columns 2 thru 7 is identical to the order in the minor edits.

TOPAZ users may employ a variety of available plot packages to read and process the plot file. The interactive SNLL code CPLOT, written by M. L. Chiesa, 8241 and M. L. Callabresi, 8242 is ideally suited for this purpose since the 7E13.4 format is the default format for CPLOT. CPLOT is not formally documented although instructions are given on line during the interactive execution.

V. CONCLUDING COMMENTS

TOPAZ and the numerical integrator DASSL are relatively "robust" codes, but from time to time users (especially new users) will pose gas transfer problems which cause the integrator to fail. Usually these problems can be overcome by opening valves more slowly, changing the spacial discretization along the flow path (i.e. changing the number of CE's in the PIPE's), or relocating valves in the network. In nearly all cases such changes do not significantly affect the solution to the problem for the time scales of interest. As a last resort, users may consider altering the DASSL time intergration error tolerances RTOL and ATOL (particularly ATOL).

When all else fails users are encouraged to contact the author for advice whenever severe problems arise. Efforts will continue to be made to increase the "robustness" of the code, however, it is anticipated that the most significant code improvements will be a direct result of user's comments and feedback.

VI. REFERENCES

1. W.S. Winters, "TOPAZ-A Computer Code for Modeling Heat Transfer and Fluid Flow in Arbitrary Networks of Pipes, Flow Branches, and Vessels," SAND83-8253, Sandia National Laboratories, Livermore, CA, January 1984.
2. W.S. Winters, "DRAC-User Friendly Computer Code for Modeling Transient Thermohydraulic Phenomena in Solar Receiver Tubing," SAND82-8744, Sandia National Laboratories, Livermore, CA, January 1983.
3. W.S. Winters and M.P. Kanouff, "Implementation of Empirical Total Pressure Loss Data into the DUCTFLO and TOPAZ Gas Transfer Codes," SAND84-8246, Sandia National Laboratories, Livermore, CA, November 1984.
4. L.R. Petzold, "A Description of DASSL: A Differential/Algebraic System Solver," SAND82-8637, Sandia National Laboratories, Livermore, CA, September 1982.
5. W.S. Winters, "TOPAZ - The Transient One-Dimensional Pipe Flow Analyzer: User's Manual," SAND85-8215, Sandia National Laboratories, Livermore, CA, July, 1985.
6. P.J. Roache, "Computational Fluid Dynamics," Hermosa Publishers, Albuquerque, NM, p. 237, 1976.

 

APPENDIX A - Further Discussion of EXAMPLE 3

The purpose of this appendix is to present and discuss the output from TOPAZ modeling of EXAMPLE 3. The first page of TOPAZ output is a header page, identifying the code name, the author, and the units assumed (SI) for input and output data. The second page of output is an echo of the user's input file. In this example the information listed in Table 8 or 9 would appear on the second page of the TOPAZ output.

Pages 3 thru 5 of EXAMPLE 3 output contain the User/TOPAZ mesh generation Table. This table is reproduced here as Table 10. The User/TOPAZ Mesh Generation Table will be printed whenever the LIST=1 (default) option is used. This table is extremely useful since it identifies the correspondence between the user component numbering and the numbering of the CEs and Ms in the TOPAZ finite difference mesh. This information can be useful in interpreting the major and minor edits since these edits are labeled using the CE and M numbering.

Variables associated with CHAMBERS, JOINTs and PISTONs components are easily identified in the edits since the user component numbering is identical to the numbering of CE, M, and PISTON elements by the TOPAZ mesh generator. However, the mesh generation table is almost always required in identifying the CE and M numbers associated with PIPEs.

In this example the PIPE was divided into 20 equally sized CEs. The mesh generation table for the problem shows that the CEs and Ms for this component (PIPE=5) are numbered consecutively from 5 to 43. Numbering of CE and M elements within PIPE components always begins at the upstream end and proceeds toward the downstream end. With this knowledge and with the User/TOPAZ Mesh Generation Table, the user is in a position to print out a considerable amount of data for any location in the pipe. For example, if the user is interested in printing properties at the middle of the PIPE, minor edits can be performed on CE number 23, the CE at that location.

The mesh generation table is also useful for checking the initial conditions for the problem. The initial temperature, pressure, number of moles, mole fractions and volumes are printed for all CEs in the simulation.

Two smaller tables appear after the mesh generation table. The first of these tables identifies the JOINTs which act as valves during the simulation. In this example the table entitled "VALVE OPENING AND CLOSING INFORMATION" reminds the user that JOINT number 3 has been designated as a valve which starts to open at TIME=0. and starts to close at TIME=.25. The times required to open and close are also printed (.005 seconds) in this table. The second of the two tables, entitled "MINOR EDIT INFORMATION", reminds the user which elements (CE, M, or PISTON elements) and which properties were selected for minor edits.

Table 10. User/TOPAZ Mesh Generation Table for EXAMPLE 3

THE FOLLOWING USER-TOPAZ MESH INFORMATION IDENTIFIES THE CORRESPONDENCE BETWEEN USER COMPONENT NUMBERING (I.E. THE NUMBERING OF JOINTS, CHAMBERS, PISTONS, AND PIPES) AND THE MESH GENERATOR NUMBERING OF TOPAZ MOMENTUM ELEMENTS (M), CONTINUITY-ENERGY ELEMENTS (CE), AND PISTON ELEMENTS (P). THE INITIAL PRESSURES, TEMPERATURES, GAS COMPOSITIONS, AND EQUATION OF STATE NUMBER (EOS) ARE LISTED FOR ALL TOPAZ CE ELEMENTS. INFORMATION ON VALVE TIMING, AND EDITS FOLLOW.

COMPONENT/ELEMENT NUMBERING				INITIAL CONDITIONS APPLICABLE TO CONTINUITY-ENERGY ELEMENTS									
COMPONENT TYPE	COMP NUMB	ELEMENT TYPE	ELEMENT NUMB	TEMPERATURE DEGREES - K	PRESSURE PA=N/SQM	EOS	TOTAL MOLES	MOLE FRACTION OF EACH SPECIES N, WHERE N = 1, 2, 3, 4, 5					VOLUME M CUBE
CHAMBER	1	CE	1	2.950e+02	1.79e+07	2	7.459e-04	0.665	0.000	0.000	0.000	0.335	1.131e-04
CHAMBER	2	CE	2	2.950e+02	6.89e+03	2	3.531e-05	1.000	0.000	0.000	0.000	0.000	1.257e-02
JOINT*	3	M	3										
JOINT	4	M	4										
PIPE	5	CE	5	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	6										
		CE	7	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	8										
		CE	9	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	10										
		CE	11	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	12										
		CE	13	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	14										
		CE	15	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	16										
		CE	17	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	18										
		CE	19	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	20										
		CE	21	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	22										
		CE	23	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	24										
		CE	25	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	26										
		CE	27	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	28										
		CE	29	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	30										
		CE	31	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	32										
		CE	33	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	34										
		CE	35	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	36										
		CE	37	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	38										
		CE	39	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	40										
		CE	41	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07
		M	42										
		CE	43	2.950e+02	6.89e+03	2	9.931e-10	1.000	0.000	0.000	0.000	0.000	3.534e-07

* DESIGNATES JOINTS (VALVES) WHICH OPEN AND/OR CLOSE DURING THE SIMULATION.

Table 10. Continued

JOINT OPENING AND CLOSING INFORMATION

JOINT 3 IS A VALVE OPENING AT TIME=0. TIME REQUIRED TO OPEN=5.000e-03
JOINT 3 IS A VALVE CLOSING AT TIME=2.500e-01 TIME REQUIRED TO CLOSE=5.000e-03

MINOR EDIT INFORMATION

MINOR EDIT FREQUENCY=1.000e-02 SECONDS

AT CONTROL VOLUME	1 MINOR EDIT VARIABLE IS MIXTURE PRESSURE
AT CONTROL VOLUME	1 MINOR EDIT VARIABLE IS MIXTURE TEMPERATURE
AT CONTROL VOLUME	2 MINOR EDIT VARIABLE IS MIXTURE PRESSURE
AT CONTROL VOLUME	3 MINOR EDIT VARIABLE IS MIXTURE MASS FLOW RATE
AT CONTROL VOLUME	2 MINOR EDIT VARIABLE IS MASS OF GAS SPECIES 1
AT CONTROL VOLUME	2 MINOR EDIT VARIABLE IS MASS OF GAS SPECIES 5

The remaining pages of the TOPAZ output file consist of the user requested major and minor edits (printouts of the dependent variables as a function of time). Table 11 contains the major and minor edits for EXAMPLE 3. Major edits are enclosed by a border of asterisks in order to distinguish them from the minor edits. The major edit is a printout of the pressure at all CE elements, the velocity at all M elements, and the displacement at all PISTON elements. Major edits usually require more than one line in the output file. In this example, 10 lines were required for major editing (8 for data and 2 for the border). The major and minor edit frequencies specified in the input file have resulted in the interspersing of 10 minor edits between each major edit.

The output file also identifies the locations and times for flow choking and unchoking in addition to messages regarding piston movement. In this example the messages indicate that choking and unchoking have occurred at momentum element 4, i.e. JOINT 4 at the entrance to the receiver. This is the location one would expect, since it is the area of rapid flow expansion in the flow path. Choking occurs almost immediately ($TIME=1.037946e-03$) after opening the valve. The flow remains choked at that point until the $TIME=2.066529e-01$ seconds when the local pressure ratio falls below the critical value.

Figures 1 thru 6 are plots of the 6 minor edit variables as a function of time. The data used in making the plots was available in the TOPAZ generated plot post process file and the plots were generated using CPLOT.

The reservoir pressure transient is shown in Figure 1, and the corresponding reservoir temperature is shown in Figure 2. The temperature in the reservoir falls rapidly due to the gas expansion until $TIME=.25$ seconds when the valve linking the reservoir to the receiver begins to close. At that point heat transfer from the surrounding reservoir walls begins to heat the reservoir gas causing the observed temperature rise.

The pressure, hydrogen inventory, and helium inventory for the receiver is plotted in Figure 3, 5, and 6 respectively. The slight discontinuity in the curves at $TIME=.25$ seconds indicates that the receiver was not quite filled when the valve was closed. A more obvious discontinuity is apparent in the plot of valve mass flow rate of Figure 4. Closure of the valve between .25 and .255 seconds is clearly evident in the plot.

Table 11. Major and Minor Edits for EXAMPLE 3

```

TIME= 0.          P( 1)= 1.791e+07 T( 1)= 2.950e+02 P( 2)= 6.895e+03 W( 3)= 0.          M1( 2)= 7.118e-05 M5( 2)= 0.

*****TIME= 0.*****
* P( 1)= 1.791e+07 P( 2)= 6.895e+03 V( 3)= 0.          V( 4)= 0.          P( 5)= 6.895e+03 V( 6)= 0.          *
* P( 7)= 6.895e+03 V( 8)= 0.          P( 9)= 6.895e+03 V( 10)= 0.          P( 11)= 6.895e+03 V( 12)= 0.          *
* P( 13)= 6.895e+03 V( 14)= 0.          P( 15)= 6.895e+03 V( 16)= 0.          P( 17)= 6.895e+03 V( 18)= 0.          *
* P( 19)= 6.895e+03 V( 20)= 0.          P( 21)= 6.895e+03 V( 22)= 0.          P( 23)= 6.895e+03 V( 24)= 0.          *
* P( 25)= 6.895e+03 V( 26)= 0.          P( 27)= 6.895e+03 V( 28)= 0.          P( 29)= 6.895e+03 V( 30)= 0.          *
* P( 31)= 6.895e+03 V( 32)= 0.          P( 33)= 6.895e+03 V( 34)= 0.          P( 35)= 6.895e+03 V( 36)= 0.          *
* P( 37)= 6.895e+03 V( 38)= 0.          P( 39)= 6.895e+03 V( 40)= 0.          P( 41)= 6.895e+03 V( 42)= 0.          *
* P( 43)= 6.895e+03
*****

CHOKING AT ELEMENT 4 TIME= 1.038141e-03 V= 1.3777e+03
TIME= 1.03814e-03 P( 1)= 1.781e+07 T( 1)= 2.945e+02 P( 2)= 6.895e+03 W( 3)= 3.477e-02 M1( 2)= 7.119e-05 M5( 2)= 7.312e-11
TIME= 1.00000e-02 P( 1)= 1.321e+07 T( 1)= 2.678e+02 P( 2)= 2.678e+04 W( 3)= 2.894e-02 M1( 2)= 2.075e-04 M5( 2)= 1.363e-04
TIME= 2.00000e-02 P( 1)= 1.014e+07 T( 1)= 2.463e+02 P( 2)= 4.639e+04 W( 3)= 2.247e-02 M1( 2)= 3.423e-04 M5( 2)= 2.711e-04
TIME= 3.00000e-02 P( 1)= 7.965e+06 T( 1)= 2.282e+02 P( 2)= 6.180e+04 W( 3)= 1.781e-02 M1( 2)= 4.480e-04 M5( 2)= 3.769e-04
TIME= 4.00000e-02 P( 1)= 6.382e+06 T( 1)= 2.129e+02 P( 2)= 7.411e+04 W( 3)= 1.436e-02 M1( 2)= 5.325e-04 M5( 2)= 4.614e-04
TIME= 5.00000e-02 P( 1)= 5.191e+06 T( 1)= 1.997e+02 P( 2)= 8.419e+04 W( 3)= 1.173e-02 M1( 2)= 6.016e-04 M5( 2)= 5.305e-04
TIME= 6.00000e-02 P( 1)= 4.312e+06 T( 1)= 1.885e+02 P( 2)= 9.218e+04 W( 3)= 9.767e-03 M1( 2)= 6.564e-04 M5( 2)= 5.854e-04
TIME= 7.00000e-02 P( 1)= 3.635e+06 T( 1)= 1.788e+02 P( 2)= 9.875e+04 W( 3)= 8.246e-03 M1( 2)= 7.015e-04 M5( 2)= 6.304e-04
TIME= 8.00000e-02 P( 1)= 3.094e+06 T( 1)= 1.702e+02 P( 2)= 1.043e+05 W( 3)= 7.022e-03 M1( 2)= 7.398e-04 M5( 2)= 6.688e-04
TIME= 9.00000e-02 P( 1)= 2.646e+06 T( 1)= 1.625e+02 P( 2)= 1.093e+05 W( 3)= 6.008e-03 M1( 2)= 7.736e-04 M5( 2)= 7.026e-04
TIME= 1.00000e-01 P( 1)= 2.283e+06 T( 1)= 1.556e+02 P( 2)= 1.135e+05 W( 3)= 5.179e-03 M1( 2)= 8.027e-04 M5( 2)= 7.317e-04

*****TIME= 1.00000e-01*****
* P( 1)= 2.283e+06 P( 2)= 1.135e+05 V( 3)= 1.589e+02 V( 4)= 1.068e+03 P( 5)= 2.212e+06 V( 6)= 1.833e+02 *
* P( 7)= 2.171e+06 V( 8)= 2.080e+02 P( 9)= 2.129e+06 V( 10)= 2.252e+02 P( 11)= 2.085e+06 V( 12)= 2.442e+02 *
* P( 13)= 2.039e+06 V( 14)= 2.624e+02 P( 15)= 1.990e+06 V( 16)= 2.799e+02 P( 17)= 1.940e+06 V( 18)= 2.970e+02 *
* P( 19)= 1.887e+06 V( 20)= 3.140e+02 P( 21)= 1.832e+06 V( 22)= 3.312e+02 P( 23)= 1.774e+06 V( 24)= 3.489e+02 *
* P( 25)= 1.713e+06 V( 26)= 3.674e+02 P( 27)= 1.648e+06 V( 28)= 3.872e+02 P( 29)= 1.579e+06 V( 30)= 4.088e+02 *
* P( 31)= 1.505e+06 V( 32)= 4.330e+02 P( 33)= 1.424e+06 V( 34)= 4.608e+02 P( 35)= 1.336e+06 V( 36)= 4.940e+02 *
* P( 37)= 1.235e+06 V( 38)= 5.356e+02 P( 39)= 1.117e+06 V( 40)= 5.915e+02 P( 41)= 9.665e+05 V( 42)= 6.781e+02 *
* P( 43)= 5.527e+05
*****

TIME= 1.10000e-01 P( 1)= 1.984e+06 T( 1)= 1.495e+02 P( 2)= 1.172e+05 W( 3)= 4.495e-03 M1( 2)= 8.280e-04 M5( 2)= 7.570e-04
TIME= 1.20000e-01 P( 1)= 1.738e+06 T( 1)= 1.440e+02 P( 2)= 1.204e+05 W( 3)= 3.927e-03 M1( 2)= 8.500e-04 M5( 2)= 7.790e-04
TIME= 1.30000e-01 P( 1)= 1.530e+06 T( 1)= 1.391e+02 P( 2)= 1.232e+05 W( 3)= 3.453e-03 M1( 2)= 8.692e-04 M5( 2)= 7.982e-04
TIME= 1.40000e-01 P( 1)= 1.356e+06 T( 1)= 1.348e+02 P( 2)= 1.257e+05 W( 3)= 3.054e-03 M1( 2)= 8.862e-04 M5( 2)= 8.152e-04
TIME= 1.50000e-01 P( 1)= 1.209e+06 T( 1)= 1.308e+02 P( 2)= 1.279e+05 W( 3)= 2.715e-03 M1( 2)= 9.012e-04 M5( 2)= 8.302e-04
TIME= 1.60000e-01 P( 1)= 1.083e+06 T( 1)= 1.273e+02 P( 2)= 1.298e+05 W( 3)= 2.426e-03 M1( 2)= 9.145e-04 M5( 2)= 8.436e-04
TIME= 1.70000e-01 P( 1)= 9.753e+05 T( 1)= 1.242e+02 P( 2)= 1.316e+05 W( 3)= 2.177e-03 M1( 2)= 9.265e-04 M5( 2)= 8.555e-04
TIME= 1.80000e-01 P( 1)= 8.822e+05 T( 1)= 1.213e+02 P( 2)= 1.331e+05 W( 3)= 1.963e-03 M1( 2)= 9.372e-04 M5( 2)= 8.662e-04
TIME= 1.90000e-01 P( 1)= 8.014e+05 T( 1)= 1.188e+02 P( 2)= 1.345e+05 W( 3)= 1.777e-03 M1( 2)= 9.468e-04 M5( 2)= 8.758e-04
TIME= 2.00000e-01 P( 1)= 7.307e+05 T( 1)= 1.165e+02 P( 2)= 1.358e+05 W( 3)= 1.615e-03 M1( 2)= 9.555e-04 M5( 2)= 8.845e-04

*****TIME= 2.00000e-01*****
* P( 1)= 7.307e+05 P( 2)= 1.358e+05 V( 3)= 1.142e+02 V( 4)= 1.074e+03 P( 5)= 7.151e+05 V( 6)= 1.461e+02 *
* P( 7)= 7.017e+05 V( 8)= 1.748e+02 P( 9)= 6.876e+05 V( 10)= 2.005e+02 P( 11)= 6.730e+05 V( 12)= 2.239e+02 *
* P( 13)= 6.577e+05 V( 14)= 2.452e+02 P( 15)= 6.418e+05 V( 16)= 2.651e+02 P( 17)= 6.252e+05 V( 18)= 2.840e+02 *
* P( 19)= 6.078e+05 V( 20)= 3.021e+02 P( 21)= 5.896e+05 V( 22)= 3.201e+02 P( 23)= 5.706e+05 V( 24)= 3.381e+02 *
* P( 25)= 5.505e+05 V( 26)= 3.567e+02 P( 27)= 5.292e+05 V( 28)= 3.764e+02 P( 29)= 5.066e+05 V( 30)= 3.978e+02 *
* P( 31)= 4.824e+05 V( 32)= 4.218e+02 P( 33)= 4.561e+05 V( 34)= 4.490e+02 P( 35)= 4.271e+05 V( 36)= 4.817e+02 *
* P( 37)= 3.945e+05 V( 38)= 5.227e+02 P( 39)= 3.563e+05 V( 40)= 5.783e+02 P( 41)= 3.074e+05 V( 42)= 6.649e+02 *
* P( 43)= 1.718e+05
*****

UNCHOKING AT ELEMENT 4 TIME= 2.078210e-01 V= 1.0740e+03
TIME= 2.07821e-01 P( 1)= 6.815e+05 T( 1)= 1.149e+02 P( 2)= 1.367e+05 W( 3)= 1.501e-03 M1( 2)= 9.618e-04 M5( 2)= 8.908e-04
TIME= 2.10000e-01 P( 1)= 6.686e+05 T( 1)= 1.145e+02 P( 2)= 1.370e+05 W( 3)= 1.472e-03 M1( 2)= 9.634e-04 M5( 2)= 8.924e-04
TIME= 2.20000e-01 P( 1)= 6.145e+05 T( 1)= 1.127e+02 P( 2)= 1.380e+05 W( 3)= 1.349e-03 M1( 2)= 9.705e-04 M5( 2)= 8.996e-04

```

Table 11. Continued

```

TIME= 2.30000e-01 P( 1)= 5.668e+05 T( 1)= 1.111e+02 P( 2)= 1.389e+05 W( 3)= 1.239e-03 M1( 2)= 9.770e-04 M5( 2)= 9.060e-04
TIME= 2.40000e-01 P( 1)= 5.240e+05 T( 1)= 1.097e+02 P( 2)= 1.398e+05 W( 3)= 1.140e-03 M1( 2)= 9.830e-04 M5( 2)= 9.120e-04
TIME= 2.50000e-01 P( 1)= 4.860e+05 T( 1)= 1.085e+02 P( 2)= 1.406e+05 W( 3)= 1.051e-03 M1( 2)= 9.884e-04 M5( 2)= 9.175e-04
TIME= 2.60000e-01 P( 1)= 4.779e+05 T( 1)= 1.094e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.918e-04 M5( 2)= 9.205e-04
TIME= 2.70000e-01 P( 1)= 4.870e+05 T( 1)= 1.115e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.918e-04 M5( 2)= 9.206e-04
TIME= 2.80000e-01 P( 1)= 4.960e+05 T( 1)= 1.135e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.918e-04 M5( 2)= 9.206e-04
TIME= 2.90000e-01 P( 1)= 5.049e+05 T( 1)= 1.156e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.00000e-01 P( 1)= 5.137e+05 T( 1)= 1.176e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
*****TIME= 3.00000e-01*****
* P( 1)= 5.137e+05 P( 2)= 1.411e+05 V( 3)= 0. V( 4)= 1.937e-03 P( 5)= 1.411e+05 V( 6)= 4.774e-04 *
* P( 7)= 1.411e+05 V( 8)= 8.367e-04 P( 9)= 1.411e+05 V( 10)= 1.107e-03 P( 11)= 1.411e+05 V( 12)= 1.310e-03 *
* P( 13)= 1.411e+05 V( 14)= 1.462e-03 P( 15)= 1.411e+05 V( 16)= 1.575e-03 P( 17)= 1.411e+05 V( 18)= 1.661e-03 *
* P( 19)= 1.411e+05 V( 20)= 1.725e-03 P( 21)= 1.411e+05 V( 22)= 1.773e-03 P( 23)= 1.411e+05 V( 24)= 1.809e-03 *
* P( 25)= 1.411e+05 V( 26)= 1.838e-03 P( 27)= 1.411e+05 V( 28)= 1.860e-03 P( 29)= 1.411e+05 V( 30)= 1.877e-03 *
* P( 31)= 1.411e+05 V( 32)= 1.891e-03 P( 33)= 1.411e+05 V( 34)= 1.902e-03 P( 35)= 1.411e+05 V( 36)= 1.912e-03 *
* P( 37)= 1.411e+05 V( 38)= 1.919e-03 P( 39)= 1.411e+05 V( 40)= 1.926e-03 P( 41)= 1.411e+05 V( 42)= 1.932e-03 *
* P( 43)= 1.411e+05
*****
TIME= 3.10000e-01 P( 1)= 5.224e+05 T( 1)= 1.196e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.20000e-01 P( 1)= 5.310e+05 T( 1)= 1.215e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.30000e-01 P( 1)= 5.394e+05 T( 1)= 1.235e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.40000e-01 P( 1)= 5.478e+05 T( 1)= 1.254e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.50000e-01 P( 1)= 5.561e+05 T( 1)= 1.273e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.60000e-01 P( 1)= 5.643e+05 T( 1)= 1.292e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.70000e-01 P( 1)= 5.723e+05 T( 1)= 1.310e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.80000e-01 P( 1)= 5.803e+05 T( 1)= 1.328e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 3.90000e-01 P( 1)= 5.882e+05 T( 1)= 1.346e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.00000e-01 P( 1)= 5.960e+05 T( 1)= 1.364e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
*****TIME= 4.00000e-01*****
* P( 1)= 5.960e+05 P( 2)= 1.411e+05 V( 3)= 0. V( 4)= -6.105e-09 P( 5)= 1.411e+05 V( 6)= -1.657e-09 *
* P( 7)= 1.411e+05 V( 8)= -2.899e-09 P( 9)= 1.411e+05 V( 10)= -3.827e-09 P( 11)= 1.411e+05 V( 12)= -4.519e-09 *
* P( 13)= 1.411e+05 V( 14)= -5.034e-09 P( 15)= 1.411e+05 V( 16)= -5.419e-09 P( 17)= 1.411e+05 V( 18)= -5.706e-09 *
* P( 19)= 1.411e+05 V( 20)= -5.921e-09 P( 21)= 1.411e+05 V( 22)= -6.084e-09 P( 23)= 1.411e+05 V( 24)= -6.208e-09 *
* P( 25)= 1.411e+05 V( 26)= -6.303e-09 P( 27)= 1.411e+05 V( 28)= -6.378e-09 P( 29)= 1.411e+05 V( 30)= -6.436e-09 *
* P( 31)= 1.411e+05 V( 32)= -6.483e-09 P( 33)= 1.411e+05 V( 34)= -6.521e-09 P( 35)= 1.411e+05 V( 36)= -6.553e-09 *
* P( 37)= 1.411e+05 V( 38)= -6.580e-09 P( 39)= 1.411e+05 V( 40)= -6.602e-09 P( 41)= 1.411e+05 V( 42)= -6.613e-09 *
* P( 43)= 1.411e+05
*****
TIME= 4.10000e-01 P( 1)= 6.038e+05 T( 1)= 1.382e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.20000e-01 P( 1)= 6.114e+05 T( 1)= 1.399e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.30000e-01 P( 1)= 6.190e+05 T( 1)= 1.417e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.40000e-01 P( 1)= 6.265e+05 T( 1)= 1.434e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.50000e-01 P( 1)= 6.339e+05 T( 1)= 1.451e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.60000e-01 P( 1)= 6.412e+05 T( 1)= 1.468e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.70000e-01 P( 1)= 6.484e+05 T( 1)= 1.484e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.80000e-01 P( 1)= 6.555e+05 T( 1)= 1.500e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 4.90000e-01 P( 1)= 6.626e+05 T( 1)= 1.517e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
TIME= 5.00000e-01 P( 1)= 6.695e+05 T( 1)= 1.532e+02 P( 2)= 1.411e+05 W( 3)= 0. M1( 2)= 9.916e-04 M5( 2)= 9.206e-04
*****TIME= 5.00000e-01*****
* P( 1)= 6.695e+05 P( 2)= 1.411e+05 V( 3)= 0. V( 4)= -5.733e-12 P( 5)= 1.411e+05 V( 6)= -1.792e-12 *
* P( 7)= 1.411e+05 V( 8)= -3.029e-12 P( 9)= 1.411e+05 V( 10)= -3.785e-12 P( 11)= 1.411e+05 V( 12)= -4.820e-12 *
* P( 13)= 1.411e+05 V( 14)= -5.421e-12 P( 15)= 1.411e+05 V( 16)= -5.873e-12 P( 17)= 1.411e+05 V( 18)= -6.244e-12 *
* P( 19)= 1.411e+05 V( 20)= -6.423e-12 P( 21)= 1.411e+05 V( 22)= -6.626e-12 P( 23)= 1.411e+05 V( 24)= -7.016e-12 *
* P( 25)= 1.411e+05 V( 26)= -7.102e-12 P( 27)= 1.411e+05 V( 28)= -7.331e-12 P( 29)= 1.411e+05 V( 30)= -7.598e-12 *
* P( 31)= 1.411e+05 V( 32)= -7.589e-12 P( 33)= 1.411e+05 V( 34)= -7.741e-12 P( 35)= 1.411e+05 V( 36)= -7.979e-12 *
* P( 37)= 1.411e+05 V( 38)= -8.095e-12 P( 39)= 1.411e+05 V( 40)= -8.117e-12 P( 41)= 1.411e+05 V( 42)= -8.198e-12 *
* P( 43)= 1.411e+05
*****

```

Figure 1. Reservoir pressure for EXAMPLE 3.

Figure 2. Reservoir temperature for EXAMPLE 3.

Figure 3. Receiver pressure for EXAMPLE 3.

Figure 4. Valve mass flow rate for EXAMPLE 3.

Figure 5. Receiver hydrogen inventory for EXAMPLE 3.

Figure 6. Receiver helium inventory for EXAMPLE 3.

APPENDIX B - Calculations With Sliding Pistons

From time to time TOPAZ users may wish to incorporate the motion of CHAMBER walls into gas transfer calculations. Typical examples include analysis of gas transfer networks having diaphragms, bladders, and pistons. TOPAZ models such moving boundaries using the piston element (P). During the mesh generation, P elements are connected to CE and M elements to form the TOPAZ mesh.

Input data for the piston model are communicated to TOPAZ by including PISTON component directives as part of the input file. Table 4 contains a brief description of these directives.

Use of the PISTON directives can best be explained by introducing the physical model for the PISTON. Consider Figure 7, which shows two CHAMBERS separated by a sliding PISTON. The CHAMBER on the left of the PISTON will be referred to here as the upstream (u) CHAMBER, while the CHAMBER on the right will be referred to as the downstream (d) CHAMBER. Input data for these two CHAMBERS is entered in the usual way using CHAMBER directives (Table 1.)

During the simulation, any pressure difference across the PISTON has the potential for moving the PISTON between the u and d CHAMBERS. TOPAZ accounts for the corresponding increase or decrease in CHAMBER volumes and the work associated with the PISTON movement.

The second order ordinary differential equation (B-1) is solved by TOPAZ in order to calculate the position of the piston.

$$\text{MASS} \cdot \ddot{X} + \text{CVIS} \cdot \dot{X} + \text{KSPR} \cdot (X - X_{KZE}) = \text{AFAC} \cdot \text{AREA} \cdot (P_u - P_d) - \text{FCOU} + \text{FORC} \quad (\text{B-1})$$

The notation used in the above equation is defined in Table 4.

Readers will recognize the left hand side of equation (B-1) as the classical mass-spring-damper equation. The right hand side of the equation represents the sum of external forces acting on the piston. The first term on the right hand side is the net pressure force acting on the piston. Hence the piston motion is coupled to the time dependent pressures in the upstream and downstream CHAMBERS. Users may decouple the effects of pressure by specifying a value of AFAC equal to 0. PISTON motion will still cause increases and decreases in the adjacent CHAMBER volumes providing the value of AREA is non zero.

Figure 7. The piston model.

The second term on the right is due to coulomb friction force acting on the PISTON. This force is a user specified constant and simulates the effect of sliding friction on the PISTON. This force always opposes the motion of the PISTON and is not present when the PISTON is at rest. Hence:

$$\text{COULOMB FRICTION FORCE} = \begin{cases} -\text{FCOU} & \text{for } \dot{X} < 0 \\ 0 & \text{for } \dot{X} = 0 \\ +\text{FCOU} & \text{for } \dot{X} > 0 \end{cases} \quad (\text{B-2})$$

The third term on the right hand side of equation (B-1) is a user specified constant force applied to the PISTON. The force is applied to the PISTON only for the time period between FSTA and FSTO.

Users should constrain the motion of the PISTON by specifying the position of mechanical stops. The minor directives required are XMUP, which constrains the PISTON from moving more than a user specified distance into the upstream CHAMBER, and XMDN which provides for similar constraint in the downstream direction. Users are prevented from specifying values of XMUP and XMDN which would allow the adjacent CHAMBER volumes to become less than or equal to zero.

The FBRE directive may be used to specify a "breakaway" force for the PISTON. When this directive is used, the PISTON will be held at its initial location until sufficient external and spring forces exceed the breakaway force. The user specified breakaway force has no influence on PISTON motion once the piston moves from its initial location.

The specification of upstream and downstream CHAMBER numbers is arbitrary. The initial PISTON location at time zero is always assumed to be $X=0$. If the calculated position, X , of the PISTON is positive, it implies the piston has moved into the downstream CHAMBER. Similarly, if the calculated position is negative, the piston has moved into the upstream CHAMBER.

APPENDIX C - Additional Modeling Considerations

1. Modeling Expansions and Contractions

The comprehensive example discussed Section III and Appendix A dealt with a constant diameter flow path. The available CHAMBER, PIPE, AND JOINT directives can easily be employed to model pipe ID changes, pipe bends, and orifices in the the flow path. Generally this is accomplished by placing a JOINT with the appropriate form loss characteristics at the ID change, pipe bend, or orifice. Orifices of finite length can also be modeled using extremely short pipes having an ID equivalent to the orifice ID. Orifice form loss characteristics can then be applied to the adjacent JOINTs. Limitations in modeling with "short pipes" are discussed below.

2. Networks With Flow Branching

One of the most powerful attributes of TOPAZ is its ability to model gas transfer in networks having flow branches. The major and minor directives required for such modeling have already been introduced in Tables 1 through 7.

Consider a variation on the example previously discussed in Section III and Appendix A. Suppose the single reservoir is replaced by two reservoirs, each with unique initial conditions. The outlet pipe from each reservoir and the supply pipe to the receiver meet at a "flow branch" in the piping network. Figure 8 shows how CHAMBERS, PIPES, and JOINTs, could be assembled to simulate this situation. In flow branching situations, a CHAMBER is used as a "branch volume" and JOINTs (three in this case) are used to join the PIPES which form the branch. The volume of this CHAMBER should approximate the branch volume in the actual network. Often these volumes are of the same order of magnitude as the CE volumes in adjacent PIPES. In such cases the flow will not stagnate at the branch volume as it does in the larger reservoirs and receivers. TOPAZ will account for the non stagnating flow. Users may specify cylindrical or spherical CHAMBER shapes for branch volumes. For the smallest branch volumes it is recommended that diameters of such volumes be made two or three times the diameter of the largest adjacent pipe. Form loss information associated with branch entrance and exit effects may be applied at the JOINTs adjacent to the branch volume. The user may specify as many as 6 flow paths converging at a single branch volume.

The branch modeling technique outlined here can be extended to systems of any complexity, i.e. branches on branches, tree-like configurations, etc.

Figure 8. Model for a system having a flow branch.

3. Accuracy of TOPAZ Calculations

When the proper spacial discretization is used, i.e. a sufficient number of CEs in each PIPE, TOPAZ will accurately replicate the one-dimensional-transient physics associated with gas transfer. It is highly desirable to minimize computational times by using the smallest possible number of CEs. Once having achieved a solution with a minimum number of CEs, users are encouraged to arbitrarily increase the number in order to determine the effect on the solution. If the solution is not affected in a significant way, the user can be confident that an adequated spacial discretization has been selected.

Unfortunately gas flows through piping networks are far from one-dimensional. Pressure losses in turning, expanding, and contracting flows, as well as boundary layer viscocity and heat transfer effects, all contribute important multi-dimensional effects. TOPAZ attempts to account for these effects using quasi-steady locally applied heat transfer and pressure loss models. The directives which impose these models were summarized in Tables 1 through 3.

Correlations relating to pipe flows generally assume the flow to be both quasi-steady and fully developed i.e., uninfluenced by pipe entrance and exit effects. For the time scales of interest in most problems the "quasi-steady" assumption produces negligible errors in time dependent calculations. For long pipes (e.g. pipes with length to diameter ratios in excess of say 200), the TOPAZ pipe flow correlations lead to excellent predictions without the necessity of supplying additional form loss information. However, there are two situations in which the pipe flow correlations are insufficient to produce accurate results. The first of these situations occurs for systems composed of relatively short pipes. For these systems a significant portion of the flow losses may occur in the transition flow areas (e.g. pipe entrances and exits, flow expansions, contractions, turns, etc.). The second situation occurs for systems having relatively long pipes but also one or several components with unusually large losses (i.e. comparable to the fully developed pipe flow losses). In these situations the burden of supplying appropriate loss information falls on the user. Unfortunately, such loss information is not always available in the literature and laboratory experiments may be required in order to develop the required loss models.

Another area of TOPAZ modeling uncertainty relates to the vessel heat transfer calculations. For vessels which act as reservoirs and undergo a simple uninterrupted blowdown, the default free convection vessel heat transfer correlation built into TOPAZ is quite reliable. The difficulty in predicting vessel heat transfer arises for vessels which act as receivers. To date, no reliable and widely applicable heat transfer correlation exists for this situation. This presents little difficulty for systems having receiver volumes which are several times larger than the reservoir volumes. For such situations either the isothermal assumption or the free convection heat transfer model can be used without greatly affecting the gas transfer time. However, for systems having receiver volumes less than, or of the same order as, the reservoir volumes, inaccurate transfer time predictions may result. For these systems a

significant portion of the gas transfer may occur after initial pressure equilibrium is achieved. Such systems are referred to as being "thermally pumped" since the vessel heat transfer contributes a significant driving potential for transferring the gas. In flow regimes where thermal pumping occurs, the accuracy of the gas transfer calculation can only be as good as the vessel heat transfer correlations.

TOPAZ users should always be aware that the diffusion physics of gas heat and mass transfer (i.e. axial heat conduction and mass diffusion) are not modeled by the code. These effects are seldom important for the short time scales of interest in most gas transfer situations. In the species tracking of multi-component gas mixtures, the code assumes that any gas entering an individual CE is instantaneously and uniformly distributed within that CE regardless of the volume. Most gas transfer situations are characterized by forced convective flows and a high degree of turbulent mixing, hence this assumption presents no difficulty for PIPEs and most vessels. Users should, however, be aware of the absence of diffusion modeling when simulating multi-species gas transfer into and out of extremely large CEs, e.g. plenum chambers.

One final modeling consideration worthy of mention relates to the constant wall temperature assumption used in the containment-to-gas heat transfer calculations. For most gas transfer problems of interest to SNLL, the thermal mass (i.e. product of heat capacity and density) of the gas containment structure exceeds the thermal mass of the gas by several orders of magnitude. Hence for the time scales of interest, negligible errors are introduced with the constant wall temperature assumption. An earlier version to the TOPAZ code, originally developed for Solar Central Receiver heat transfer and thermal hydraulic calculations (1) provided users with the option of modeling two-dimensional-transient heat conduction in the fluid/gas containment structures. This feature is not presently included in the current gas transfer version of TOPAZ since it was deemed unnecessary.

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