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TOPAZ – The Transient One-Dimensional Pipe Flow Analyzer: Equations and Numerics

W. S. Winters

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Equations and Numerics

W. S. Winters
Computational Mechanics Division
Sandia National Laboratories, Livermore

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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 report, the third in a series of reports documenting TOPAZ, deals exclusively with governing equations, numerical methods, and code architecture.

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NOMENCLATURE

<u>Symbol</u>	<u>Description</u>
A	Flow cross-sectional area
A_w	Wall heat transfer area
A_f	Piston pressure force multiplier factor
c	Isentropic sound speed
C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
c_v	Piston viscous damping coefficient
CE	Shorthand notation for continuity-energy control volume
D	Diameter
F	Vector of residuals
F_c	Piston Coulomb friction force
$F(t)$	Piston time dependent force
F_b	Piston breakaway force
f	Darcy friction factor
G	Mixture mass generation rate
h	Convective heat transfer coefficient
I	Geometric inertia parameter defined by equation (7)
K	Form loss coefficient, piston linear spring constant
k	Thermal conductivity
L	Length
M	Molecular weight
M	Shorthand notation for momentum control volume
m	Mass
P	Pressure

Pr	Prandtl number
q	Artificial viscosity pressure adjustment
Re	Reynolds number
S	Sign change factor
T	Temperature
T_w	Wall temperature
t	Time
u	Mixture internal energy per unit mass
V	Volume
v	Velocity
W	Mixture mass flow rate
X	Component mass fraction, piston displacement
X_{eq}	Piston equilibrium position
Y	Component mole fraction
y	Vector of dependent variables
y'	Vector of dependent variable time derivatives

Subscripts

<u>Symbol</u>	<u>Description</u>
d	Downstream
u	Upstream
J	Momentum control volume number
I	Continuity-energy control volume number
N	Species number
I, N	Species N at control volume I
I, J	Species N at control volume J

Greek symbols

<u>Symbol</u>	<u>Description</u>
ϵ	Tube wall roughness
μ	Viscosity
ρ	Density
ξ	Reversible pressure loss

I. INTRODUCTION

This report is the third in a series of reports documenting the computer code TOPAZ (Transient One-dimensional Pipe flow AnalyZer). The first report, reference [1], is a user's manual for the code. The second report, reference [2], presents a series of examples designed to aid users in creating TOPAZ input files. The examples selected for reference [2], were intended to demonstrate the full spectrum of TOPAZ capabilities. In addition, the example calculations provide a measure of code validation through comparisons with analytical solutions.

The purpose of this report is threefold:

1. To provide a detailed description of equations used in TOPAZ mathematical modeling
2. To provide a general description of the numerical techniques used in solving the TOPAZ equations
3. To provide an overall view of TOPAZ code architecture

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. The inherent multidimensional effects associated with flows in such networks are modeled using locally applied correlations for pressure drop and wall heat transfer. In addition to modeling a variety of internal compressible flow situations, users have the option of including the effects of moving solid boundaries such as sliding pistons, diaphragms, and rolling bladders.

Development of the first version of TOPAZ at SNLL was motivated by the need to model thermohydraulic phenomena in solar central receivers (see *e.g.* references [3, 4]). Modeling of receiver flows required the treatment of both compressible (air, steam, etc.) as well as incompressible (*e.g.* liquid sodium, molten salt, etc.) flows. Furthermore, the one-dimensional-transient flow calculations had to be coupled to two-dimensional-transient heat conduction calculations in flow containment (*i.e.* vessel and pipe walls). An assortment of boundary conditions suitable for solving solar central receiver problems were also included in the coding for the original version of TOPAZ.

The first version of TOPAZ was useful in analyzing a variety of both solar and nonsolar problems (see *e.g.* reference [5]). However, the code had two major drawbacks. First of all, the code was difficult to use. Users modeling specific flow configurations were required to write their own mesh generation/driver program. Depending on the complexity of the flow

geometry, this could become a difficult task. The code DRAC (Dynamic Receiver Analysis Code) documented in reference [4], was the first user friendly mesh generation/driver program for TOPAZ. DRAC permitted users to model a frequently encountered receiver flow situation but the code was by no means a general user interface for TOPAZ. The second major drawback to the original version of TOPAZ was the absence of a multi-species gas flow modeling capability. This was a significant limitation since a large class of problems of interest to SNLL involve gas transfer in networks where the gas composition varies as a function of position and time.

The present version of TOPAZ was designed to overcome the drawbacks of the previous version. A highly general "user friendly" interface has been developed which permits users to model complex gas transfer situations with little knowledge of compressible flow, finite differences, and implicit numerical techniques. In addition, the code has the capability of treating gas mixtures having from one to five individual species.

This document will discuss in some detail the numerical modeling for the present version of TOPAZ. Readers familiar with reference [5] will notice similarities in the material presented here and in that document. The present version of TOPAZ retains the original spacial finite difference technique (first order upwind differencing on a "displaced mesh") and the original implicit numerical techniques for integrating the equations in time (DASSL, see *e.g.*, reference [6]). Unlike the previous version, the present version treats only compressible flows. Incompressible flow modeling may be added to the code in the future if the need arises. The modeling of heat conduction in the containment has been eliminated since it is seldom, if ever, needed in gas transfer analysis. However, TOPAZ modeling has been expanded to include analysis of sliding pistons, diaphragms, and bladders.

Section II of this report will discuss the "TOPAZ modeling philosophy". The gas transport equations will be presented in Section III. The equations for modeling moving containment boundaries such as piston, bladders, etc., will be discussed in Section IV. Section V contains a brief discussion of the implicit numerical methods used to integrate the TOPAZ equations in time. The overall organization of the code will be discussed in Section VI. Several concluding remarks will be presented in Section VII. This document will not discuss how to use TOPAZ. Nor will it provide verification of the code's accuracy. These subjects are treated in the two companion documents, references [1] and [2].

II. TOPAZ CODING AND MODELING PHILOSOPHY

Numerical solution of the three-dimensional transient multi-species compressible flow conservation equations is not a practical method for analyzing gas transfer systems. Even the most powerful computing facilities are inadequate when it comes to numerically solving the complete equations for all but the simplest gas transfer systems.

The current state-of-the-art in modeling flow through complex piping networks was established several years ago by the nuclear power industry in an effort to model the postulated reactor loss of coolant accident (LOCA). Included in the large family of LOCA codes are RETRAN [7], a code developed under private funding through EPRI, and RELAP [8, 9] a set of codes developed primarily through NRC funding. With the exception of RELAP5 [9], these codes deal exclusively with equilibrium water-steam flows. RELAP5 has been extended to treat nonequilibrium water-steam flows.

The modeling philosophy used in developing TOPAZ is similar to that evolved during the development of the LOCA codes. No attempt is made to solve the complete three-dimensional-transient flow conservation equations. Instead, flows through pipes and other components are modeled as being one-dimensional and transient. The spacial dimension of interest is the axial position along the flow path. The state of the gas at a particular axial location is presumed to be uniform and representative of an "averaged" thermodynamic state over the flow path cross-section. Such a treatment would be precise if all pipe flows were "one-dimensional". Unfortunately flows through piping networks are never completely one-dimensional. Wall friction and heat transfer, area expansions and contractions, tube bends, and flow branches all have the potential for introducing significant multidimensional effects. In TOPAZ and in the LOCA codes these multidimensional effects are modeled using locally-applied flow correlations for heat transfer and pressure drop. For the most part, steady flow correlations such as the Moody friction factor correlation [10] and numerous heat transfer correlations (*e.g.* references [11, 12]) are used. Steady correlations are used for two reasons. First of all, unsteady correlations for pressure drop and wall heat transfer are practically nonexistent. Secondly, for most gas transfer problems of interest, flows are "quasi-steady".

The modeling described above is well-suited for analyzing networks having flow paths consisting of "long" relatively straight tubes. In such systems the flow becomes fully developed over most of the flow path and multidimensional effects can be modeled by the existing quasi-steady pressure drop and heat transfer correlations for tube flow. In networks where the flow path is characterized by relatively short tubes and numerous turns, branches, expansions, and contractions, the accuracy of the modeling depends on the code user's ability to specify the correct locally applied correlations. Further modeling limitations may arise in networks where significant "thermal pumping" occurs as a result

of vessel heat transfer. These and other modeling considerations are discussed in some detail in Appendix C of the User's Manual [1].

The basis for flow modeling in TOPAZ is the application of the one-dimensional, transient compressible flow conservation equations. These equations consist of conservation relationships for flow continuity, energy, and momentum. Mathematically, each of the three conservation equations is a partial differential equation with time and space (axial displacement along the flow path) as independent variables. Using conventional finite difference techniques, these three partial differential equations are replaced with a larger set of ordinary differential equations (ODEs). This technique is commonly referred to as the "method of lines". The gas flow ODEs along with the ODEs used to describe wall boundary movement (piston, diaphragms, etc.) form the complete TOPAZ mathematical model of the flow network. Solution of the TOPAZ ODEs (*i.e.* integration of the equations in time) is accomplished using the implicit differential-algebraic solver DASSL [6]. Details of this modeling procedure are discussed in subsequent sections.

III. GAS TRANSPORT EQUATIONS

1. Introduction

The purpose of this section is to present and discuss the spatially discretized finite difference equations for flow continuity, energy, and, momentum. The method used in subdividing arbitrary gas transfer systems into finite difference networks will also be discussed. The detailed steps required to convert the flow conservation partial differential equations into the spatially discretized finite difference equations (TOPAZ ODEs) will not, however, be presented. These steps are rigorously outlined in numerous references including [7] and [8].

The basic assumptions used in TOPAZ modeling of gas flow may be summarized as follows:

1. Gas flow is treated as one-dimensional and transient.
2. Flow is compressible with all local gas properties a function of the local thermodynamic state. Both real and ideal gas mixtures are modeled.
3. Axial heat conduction in the flowing gas is neglected.
4. Spatial diffusion of individual gas species is neglected.
5. Gas flows are nonreacting.
6. Body forces due to gravity and acceleration of reference frame (*i.e.* moving gas transfer networks) are neglected.
7. Temperature of the fluid containment (interior pipe and vessel walls) is assumed constant.
8. Multidimensional transient effects associated with convective heat transfer from the containment to the flowing gas are accounted for with quasi-steady locally applied heat transfer correlations.
9. Multidimensional transient effects associated with pipe wall flow friction are accounted for using quasi-steady friction factor correlations.
10. Multidimensional transient effects associated with changes in flow direction (restrictions, branches, tube bends, expansions, contractions, etc.) are accounted for using quasi-steady, locally applied form loss correlations.

11. Local mass generation is permitted if appropriate.

The significance of these assumptions will be discussed as the equations are presented.

Consider the gas transfer network schematically represented in Figure 1. The system consists of three relatively large vessels connected to each other by three tubes and a flow branch. Except for one of the tubes, all tubes are straight and have a constant inside diameter. The objective is to model the flow of gas mixtures through such a system as a function of space and time. Although the application of TOPAZ is by no means restricted to the system geometry of Figure 1, this system illustrates the basic features of the flow modeling.

The first step in modeling such a network is to subdivide the network into a large number of individual control volumes. Figure 2 illustrates how this subdivision (spacial discretization) would probably occur for the system in Figure 1. The three vessels and the branch volume are represented by single control volumes while the pipes connecting the vessels are represented by long chains of control volumes.

TOPAZ employs a displaced mesh to discretize the three flow conservation equations. This discretization requires that local continuity and energy equations be written for each and every control volume. The discretized momentum equations are then applied at the interfaces between adjacent control volumes. Hence, the locations where the momentum equations are applied are "displaced" from the locations where the continuity and energy equations are applied. The displaced mesh scheme outlined here is similar to those outlined in references [7-9]. The scheme lends itself readily to the treatment of branched flows and under some situations yields a more numerically tractable set of equations (see *e.g.* reference [13]).

For the purposes of discussion, we shall refer to the locations where the continuity and energy equations are applied as "continuity-energy" control volumes (abbreviated as CEs). The CEs for system of interest are represented by the boxes and rectangles shown in Figure 2. The locations where the momentum equations are applied will be referred to as "momentum" control volumes (abbreviated as Ms). The Ms are not clearly outlined in Figure 2, although their centers coincide with the interfaces between adjacent CEs.

Figure 2 can be used to illustrate several characteristics of the TOPAZ spacial discretization scheme:

1. All Ms connect two and only two CEs.
2. A CE may have several Ms attached to it. (Note the vessel CEs, the pipe CEs, and the branch CE have 1, 2, and 3 Ms attached to them respectively.) Actually, TOPAZ is coded to permit from 0 to 6 Ms to be attached to a given CE.
3. The boundaries or end points for all flow branches terminate in a CE. For the system in Figure 1, Figure 2 indicates that these boundary CEs are vessels.

Figure 1. Typical gas transfer network

Figure 2. Typical gas transfer network subdivided into CEs

Figure 3 shows in more detail the relationship between adjacent CEs and Ms. The nomenclature shown in the figure will be utilized in presenting the TOPAZ spacially discretized flow conservation equations.

Three adjacent CEs are shown in the Figure 3. For convenience these three CEs are labeled I-1, I, and I+1. The CE labeled I, for example, is bounded by the lines connecting the points 1-2-3-8-9-10-1. The continuity and energy equations presented here will be written for this "typical" CE.

The interface between the CEs correspond to centers of momentum control volumes. In Figure 3 these M centers are labeled J-1, J, J+1. The momentum control volume labeled J is, for example, bounded by the lines connecting points 2-3-4-5-6-7-8-9-2. Note that the lines which form the boundaries of momentum control volume J correspond to the centers of the adjacent CEs. This is, in general, true for all Ms. The momentum equation presented here will be written for the momentum control volume J. Note that this momentum control volume corresponds to a location where the cross-sectional flow area expands.

2. Species Continuity Equations

In general it is assumed that gas flowing in a network is composed of $N_{\max}$ species. Presently TOPAZ permits a maximum of 5 species, hence $N_{\max}=5$. However, the equations presented here can be extended to mixtures having any number of species. The continuity relationship for the flowing gas mixture occupying a typical continuity-energy control volume I (see Figure 3) may be expressed by the following set of equations:

$$\frac{dm_{I,N}}{dt} = \sum_{J=1}^{J_{\max}} S_J X_{J,N} W_J + X_{I,N} G_I, N = 1, 2, \dots, N_{\max} \quad (1)$$

The symbols in the above $N_{\max}$ equations are defined as follows:

- $m_{I,N}$ = The mass of species N in CE number I
- $X_{J,N}$ = The mass fraction of species N at the J cross-section
- $X_{I,N}$ = The mass fraction of species N in CE number I
- W_J = The total mass flow rate at the J cross-section
- S_J = +1 for flows entering CE number I
= -1 for flows exiting CE number I
- G_I = The total mass generation rate in CE number I
- $J_{\max}$ = Total number of CE inlets and outlets

Figure 3. TOPAZ displaced finite difference mesh

Simply stated, equation set (1) says that the time rate of change of mass of any species N within CE number I is equal to the net rate of species N mass entering and leaving the CE plus the rate at which species N is generated within the CE.

Except for special circumstances outlined in references [1, 2] the quantity G_I is taken as zero. In Figure 3, the quantity $J_{\max}$ is clearly 2, *i.e.* mass flows in and out of CE number I at two locations. This is true for all CEs which form pipes or flow paths. As mentioned previously, however, $J_{\max}$ may vary from 0 to 6 for CEs acting as vessels or branch volumes. Hence the equation set (1) may have as many as six terms of the form $S_J X_{J,N} W_J$ on the right hand side.

Gas thermodynamic properties at CE interfaces (*e.g.* those interfaces labeled J-1, J, and J+1 in Figure 3) are assumed to be identical to the “upwind” CE properties. In equation set (1) as it applies to Figure 3, this means that $X_{J,N}$ is equal to $X_{I-1,N}$. As discussed in the following sections, this upwinding of properties also extends to total mixture density, enthalpy, kinetic energy, pressure, sonic velocity, etc.

3. Mixture Energy Equation

The energy relationship of the typical CE number I is expressed as a single mixture total energy equation, *i.e.*,

$$\frac{d}{dt} \left[m \left(u + \frac{v^2}{2} \right) \right]_I = \sum_{J=1}^{J_{\max}} S_J W_J \left[u + \frac{v^2}{2} + \frac{P}{\rho} \right]_J + h A_w (T_w - T_I) - P_I \frac{dV}{dt} \quad (2)$$

The symbols in equation (2) are defined as follows:

- m = Mixture total mass
- u = Mixture internal energy per unit mass
- $v^2/2$ = Mixture kinetic energy per unit mass
- P = Mixture pressure
- ρ = Mixture density
- V = Mixture volume
- T = Mixture temperature
- T_w = Containment local wall temperature
- h = Local convective heat transfer coefficient
- A_w = Containment local surface area

The quantities S_J and W_J have previously been defined and the subscripts I and J refer to CE and CE interface quantities respectively.

Equation (2) states that the time rate of change of total mixture energy in CE number I is equal to the net energy and flow work convected into and out of the CE plus the net heat transferred from the containment to the CE minus the work done on the surroundings as a result of a moving CE solid boundary. With few exceptions (see next section) the gas containment structure is rigid with non-moving walls hence the last term in the energy equation is zero. Because of the previously mentioned upwinding of gas properties for CE interfaces, convected properties u , $v^2/2$, and P/ρ at interface J are identical to the corresponding properties in the upwind CE.

The total mass of the mixture in a given CE may be determined from the local mass fractions of each species using the following relationship:

$$m_I = \sum_{N=1}^{N_{\max}} m_{I,N} \quad (3)$$

The local mass fraction for each species is determine dividing the local mass of each species by the total local mass, *i.e.*,

$$X_{I,N} = \frac{m_{I,N}}{m_I} \quad N = 1, 2, \dots, N_{\max} \quad (4)$$

The total density of a mixture in a given CE may be determined from the CE mass and its volume, *i.e.*,

$$\rho_I = \frac{m_I}{V_I} \quad (5)$$

4. Mixture Momentum Equation

The mixture momentum equation, as it applies to the J interface in Figure 3 may be expressed as follows:

$$\begin{aligned} I_J \frac{dW_J}{dt} = & P_I - P_{I+1} + (\rho v^2)_I - (\rho v^2)_{I+1} - \left[\left(\frac{fL}{2D} \right) \frac{\rho v |v|}{2} \right]_I \\ & - \left[\left(\frac{fL}{2D} \right) \frac{\rho v |v|}{2} \right]_{I+1} \\ & - \left[K \frac{\rho v |v|}{2} \right]_J - \xi + q_I - q_{I+1} \end{aligned} \quad (6)$$

Equation (6) represents a momentum balance on the gas control volume bounded by a line connecting the points 2-3-4-5-6-7-8-9-2. The momentum balance at J involves properties from the upwind CE labeled I and the downwind CE labeled I+1. Unlike the spatially discretized continuity and energy equations, equation (6) is a central difference equation for the interface J. Details regarding the development of equation (6) are given in a number of references including [7, 8].

Previously undefined symbols in equation (6) are:

- L = CE axial length dimension
- I_J = A geometric inertia parameter
- D = Diameter
- v = Local gas mixture velocity
- f = Local Darcy friction factor
- K = Local irreversible form loss coefficient
- ξ = Reversible loss term
- q = Pressure adjustment term used to induce numerical artificial viscosity

The geometric inertia parameter is determined from the geometry of the adjacent CEs, *i.e.* the CE length, L , and CE cross-sectional area, A .

$$I_J = \frac{1}{2} \left(\frac{L_I}{A_I} + \frac{L_{I+1}}{A_{I+1}} \right) \quad (7)$$

The local gas mixture velocity is determined from the local density, mixture mass flow rate, and flow cross-sectional area as

$$v = \frac{W}{\rho A} \quad (8)$$

As discussed in the next section, the empirical quasi-steady Moody friction factor correlation [10] is usually used to calculate f . Users may also specify their own constant values for f .

The irreversible form loss coefficient, K , is used to account for local irreversible pressure losses caused by flow turning, expansion, contraction, and in general all irreversible losses not accounted for by the pipe flow friction terms. In general, the irreversible form loss term is not important for one-dimensional fully developed flow through constant diameter flow paths.

The reversible form loss term, ξ , is used to account for reversible pressure losses near the location of a sudden flow path cross-sectional area change. For real flow systems the reversible pressure losses are negligible compared to the irreversible pressure losses. However, when isentropic flows are being modeled as is frequently done for code validation cases (*e.g.* reference [2]), TOPAZ automatically includes the ξ term at all area changes. The method used to calculate ξ is outlined in references [7] and [8].

The pressure adjustment terms q_I and q_{I+1} are seldom, if ever, used in TOPAZ calculations. Their primary purpose is to reduce or eliminate numerical dispersion errors resulting from finite differencing across steep gradients such as shocks. The formulation of these terms in TOPAZ is discussed in references [2] and [14].

5. Constitutive and Property Equations

It is sometimes useful to associate a particular conservation equation with a particular flow variable in order to determine the additional constitutive and property variables required to complete the flow model. With this in mind, one can associate the energy equation (2) with the local gas mixture internal energy u_I . The species continuity equations (1) together with equations (3) through (5) give rise to the local mixture density ρ_I . The local species masses $m_{I,N}$ $N = 1, 2, \dots, N_{\max}$ calculated from equation set (1) and the molecular weight M_N for each species may be used to calculate the local mole fractions for all species, *i.e.*,

$$Y_{I,N} = \frac{m_{I,N}}{M_N} \left(\sum_{N=1}^{N_{\max}} M_N m_{I,N} \right)^{-1} \quad N = 1, 2, \dots, N_{\max} \quad (9)$$

The vector of local species mole fractions $Y_{I,N}$, $N = 1, 2, \dots, N_{\max}$ together with the local mixture density, ρ_I , and internal energy, u_I , uniquely determine the local thermodynamic state of the mixture. Hence the following required mixture thermodynamic properties and transport properties may be determined:

$$\text{Pressure: } P_I = P(\rho_I, u_I, Y_{I,N}) \quad (10)$$

$$\text{Temperature: } T_I = T(\rho_I, u_I, Y_{I,N}) \quad (11)$$

$$\text{Enthalpy: } h_I = h(\rho_I, u_I, Y_{I,N}) \quad (12)$$

$$\text{Specific heat at constant volume: } C v_I = C v(\rho_I, u_I, Y_{I,N}) \quad (13)$$

$$\text{Specific heat at constant pressure: } Cp_I = Cp(\rho_I, u_I, Y_{I,N}) \quad (14)$$

$$\text{Isentropic sound speed: } c_I = c(\rho_I, u_I, Y_{I,N}) \quad (15)$$

$$\text{Viscosity: } \mu_I = \mu(\rho_I, u_I, Y_{I,N}) \quad (16)$$

$$\text{Thermal conductivity: } k_I = k(\rho_I, u_I, Y_{I,N}) \quad (17)$$

Another important quantity appearing in the mixture energy and momentum equations is the CE velocity (*e.g.* v_{I-1}, v_I, v_{I+1} , etc). Because of the displaced mesh, the only direct calculation for velocity occurs at the CE interfaces. The mixture momentum equation (6) is used to calculate the interface mass flow rate (*e.g.* W_{J-1}, W_J, W_{J+1} , etc.) and the following equation is used to calculate the corresponding velocity:

$$v = W/A\rho \quad (18)$$

In order to determine CE local mass flow rates and velocities, it is necessary to extrapolate mass flow rate information from the CE interfaces. The equation used to calculate the CE mass flow rate from interface mass flow rates takes the following form:

$$W_I = \frac{1}{2} \left[\left(\sum_j W_J \right)_{\text{in}} + \left(\sum_J W_J \right)_{\text{out}} \right] \quad (19)$$

This interpolation is suggested in a number of references [7, 8]. It assumes that the CE mass flow rate is the average of the sum of the total mass flow rates into the CE plus the sum of the total mass flow rates out of the CE. For the most frequently encountered case in which the CE has one inflow and one outflow (*e.g.* CEs in pipes), equation (19) merely states that the mass flow rate at the center of the CE is determined through a linear interpolation of the interface mass flow rates. Once having determined the CE mass flow rates, the CE velocities may be determined from a direct application of equation (18).

The only remaining relationships required to complete the TOPAZ flow model are the correlations for h , f , and K . The following correlations are currently available for h , the heat transfer coefficient:

1. Adiabatic flow, $h=0$.
2. Isothermal flow, $h=\text{infinite}$.

3. Forced convection interior tube flow, $h = f(Re, Pr)$ based on the Dittus-Boelter heat transfer correlation [11].
4. Vessel interior wall forced/free convection, $h = f(Ra, Re)$ based on the Means and Ulrich vessel heat transfer correlation [12] as modified by Meyer [15].

The following familiar expression for the friction factor, f , in terms of the local Reynolds number, Re , is used for laminar flow situations (see *e.g.* [16]):

$$f = 64/Re \quad (20)$$

The basis for the turbulent friction factor correlation, is the empirical data of Moody [10] which was mathematically represented by Colebrook and White [17] in terms of the interior tube roughness, ϵ , the tube diameter, D , and Re using the following equation:

$$\frac{1}{\sqrt{f}} = 1.74 - 2.0 \log \left(\frac{\epsilon/D}{3.7} + \frac{2.51}{Re\sqrt{f}} \right) \quad (21)$$

The actual procedure for calculating f , in TOPAZ is identical to the method suggested by Churchill [18]. Churchill obtained a set of explicit algebraic equations for f which not only eliminated the need to solve the implicit expression (21), but also provided for a numerically smooth transition between the laminar f and the turbulent f .

Values for the form loss coefficient, K , are generally specified by the TOPAZ user. A number of references including [19, 20, 21], are available for estimating K in flow networks. Most of the published K values are valid for low Mach number ($Ma < 0.3$) or nearly incompressible flows. Furthermore, the list of K values obtainable from the literature is by no means complete, even for incompressible flows. This situation seldom gives rise to modeling problems for networks composed primarily of “long pipes” in which the bulk of the pressure losses are due to pipe wall friction. However, it should be remembered that the TOPAZ flow conservation equations are transient and one dimensional. Proper multidimensional behavior (irreversible flow turning, branching, expansion, contraction, etc.) can only be simulated through correct specification of K . Systems with “short” pipes where losses are mostly due to such multidimensional behavior may require the user to obtain precise values for K experimentally, analytically, or from the literature.

6. Flow Choking and Jet simulation Near Abrupt Area Expansions

Flow choking in TOPAZ is simulated by replacing the momentum equation (6) with the following equation:

$$W_J = \rho_J A_J c_J \quad (22)$$

where the mixture density, ρ_J , and sonic velocity, c_J , are the upwind CE values. When the flow is accelerating (W_J increasing with time) equation (22) replaces equation (6) at the point in time when v_J equals c_J . The mass flow rate, W_J , continues to be calculated using equation (22) until the right hand side of equation (6) changes sign. This marks the time when the flow begins to decelerate permitting the velocity to become subsonic.

The choked flow modeling described above mimics typical choked flow behavior. When the flow becomes choked, equation (22) prevents downstream acoustical information from propagating upstream thus decoupling the upstream and downstream flow behavior at the choke point. The author has conducted a number of numerical experiments (see *e.g.* reference [2]) which verify that the flow chokes and unchokes at the critical pressure ratio.

For steady flow it can be shown that choking can only occur at a point in the flow geometry where the flow cross-sectional area is increasing. (See, for example, Shapiro [22].) In an actual gas transfer network, however, the flow is never perfectly steady. Consider the gas transfer situation depicted in Figure 4. At time zero the valve is opened allowing the high pressure reservoir gas to flow through the two pipes and into the low pressure receiver. If the initial pressures in the reservoir and receiver are such that the critical pressure ratio is exceeded at station 1, flow choking will occur at that location. As the receiver fills, the pressure ratio at station 1 decreases below the critical value and the flow will then unchoke. However, since the flow is not perfectly steady a steep shock will quickly move upstream from station 1 to station 2 where a new choke point will be established. The time required for the shock to move between stations 1 and 2 is insignificant compared to the total transfer time. However, the TOPAZ flow equations will resolve the propagation of this shock by establishing a series of choke points in the constant diameter pipe from station 1 to station 2. Resolving this particular aspect of the flow physics contributes little to the overall accuracy of the gas transfer calculation. Furthermore, for reasons which will become apparent in Section IV, such calculations are extremely expensive from a computational time standpoint. Because of this, TOPAZ has been coded to suppress the establishment of choke points at all locations in the network where the flow cross-sectional area is not increasing. Hence in Figure 4, with the flow direction as indicated, TOPAZ will only test for choking at stations 1 and 2. This suppression of choke points in constant diameter sections of pipe does not prevent TOPAZ from identifying the correct initiation time and duration of choking at stations 1 and 2. Furthermore, it does not prevent correct identification of multiple choke points in the flow path (*e.g.* simultaneous choking at stations 1 and 2).

The simulation of unchoked flow at an abrupt increase in area often requires modeling of a subsonic jet. This is especially true when the cross-sectional area increase is so large that the flow in the downstream CE nearly stagnates. Consider, for example, the application of the momentum equation (6), at the entrance to a large receiver (*e.g.* station 1 in Figure 4). If one neglects the friction, q , and ξ terms in the momentum equation, equation (6) may be rewritten as:

Figure 4. Establishment of choke points along a flow path

$$I_J \frac{dW_J}{dt} = P_I - P_{I-1} + (\rho v^2)_I - \left(\frac{K \rho v^2}{2} \right)_J \quad (23)$$

Note that the term $(\rho v^2)_{I+1}$ has also been neglected in equation (23). The large increase in areas causes this term to become negligible compared to the $(\rho v^2)_I$ term. TOPAZ attempts to model the subsonic jet downstream of the area change by assigning a form loss factor of $K = 2$. This has the effect of reintroducing a counterbalancing ρv^2 term into the momentum equation. Attempts at modeling such expanding flows without some form of ρv^2 counterbalancing, not only results in a poor physical model (the flow immediately downstream of the J interface is not really stagnate but has considerable velocity), but also causes severe numerical difficulty. TOPAZ code users have the option of overriding the default assignment of $K = 2$ at large area changes by assigning their own values of K . For real gas transfer systems having significant pressure losses in the flow path assigning alternate values for K is seldom necessary.

IV. EQUATIONS FOR A MOVING BOUNDARY

In this section the equations for simulating the motion of pistons, diaphragms, and rolling bladders will be presented. The most general model for simulating the movement of these CE boundaries is schematically represented in Figure 5. For the purposes of discussion it shall be assumed that the CE boundary is a piston having a mass m . The piston acts as a movable wall separating two CEs referred to here as the "upstream" CE and the "downstream" CE. The piston displacement coordinate, X , is defined such that positive displacement causes the upstream CE to expand and the downstream CE to contract.

The motion of the piston is caused by differential pressure forces acting on the faces of the piston. The piston inertia, viscous damping, spring force, Coulomb friction, breakaway force, and prescribed time dependent force all affect the piston motion. The relationship between these forces and the piston motion is described by the following relationship:

$$m \frac{d^2 X}{dt^2} + c_v \frac{dX}{dt} + K(X - X_{eq}) = A_f A (P_u - P_d) - F_c + F(t) \quad (24)$$

The notation used in the equation is defined in the nomenclature.

Readers will recognize the left hand side of equation (24) as the classical mass-spring-damper equation. The right hand side represents the sum of external forces (not including the spring and viscous damping force) acting on the piston. The first term on the right hand side is the net pressure force acting on the piston. For purposes of discussion here the constant A_f is identically equal to one. (See references [1] and [2] for alternative values of A_f .) Because of the pressure force term, the piston motion is directly coupled to the thermodynamic state in the two CEs.

The second term on the right is due to Coulomb friction force acting on the piston. This force simulates the effect of sliding friction on the piston. The Coulomb friction force always opposes the motion of the piston and is not present when the piston is at rest. Hence:

$$F_c = \begin{cases} -F_c & \text{for } \dot{X} < 0 \\ 0 & \text{for } \dot{X} = 0 \\ F_c & \text{for } \dot{X} > 0 \end{cases} \quad (25)$$

The third term on the right hand side of equation (24) is a constant force (positive or negative constant acting over a user specified time period).

Figure 5. The piston moving boundary model

The piston is constrained to move between the two mechanical stops shown in Figure 5. Whenever a piston encounters a mechanical stop (*i.e.* $X = L_d$, or $X = L_u$), the velocity and acceleration terms in equation (24) are set to zero. This has the affect of freezing the piston position at the appropriate mechanical stop. The piston position remains fixed at the stop until the net force (spring, pressure, F_c , and $F(t)$) acting on the piston changes sign. This sign change indicates that there is sufficient force available to drive the piston in the opposite direction and hence off the stop.

TOPAZ users may further constrain piston motion by specifying a “breakaway” force, F_b . When a nonzero value of F_b is specified, initial piston motion will not occur unless the following condition is met:

$$F_b \leq K(X_{eq} - X) + A_f A(P_u - P_d D) - F_c + F(t) \quad (26)$$

The piston is only constrained by the breakaway force prior to the initiation of the first motion; *i.e.* the condition described by equation (26) has no importance once the piston “breaks away”.

Throughout the discussion above, the moving CE boundary has been referred to as a “piston”. Through proper specification of the appropriate constants (m, c_v, K , etc.) equation (24) may be used to simulate diaphragms, rolling bladders, etc. The equation may take the form of a second order ODE (ordinary differential equation), a first order ODE, or even a simple algebraic equation depending on which values of m, c_v , of K are set to zero.

V. SOLUTION OF EQUATIONS

The gas continuity, energy, and momentum equations together with the piston motion equations form the mathematical model for simulating flow in gas transfer systems. The dependent variables in the model include the the following quantities:

1. The mass of each gas species in each CE
2. The mixture internal energy per unit mass in each CE
3. The mixture mass flow rate at each interface (M) connecting two CEs
4. The position and velocity of each piston

The equations which form the model are a set of mixed algebraic and ordinary differential equations with time as the independent variable. With the exception of the piston motion equation (24), all ODEs naturally appear as first order ODEs. In TOPAZ the second order piston ODE is recast into two first order ODEs with piston position and velocity as the dependent variables. Hence during the solution (time integration) phase, all ODEs are first order.

Currently in TOPAZ, the set of mixed algebraic and ordinary differential model equations is solved using DASSL (Differential/Algebraic System Solver), a computer code written by L. R. Petzold [6]. DASSL is a family of Fortran subroutines and other library subroutines from LINPACK [23] and SLATEC [24], designed to perform the fully implicit numerical solution of systems of differential/algebraic equations. Only a general outline of the DASSL solution technique will be given here. No attempt will be made to describe the details of how DASSL solves the equations. For these details the reader is referred to reference [6]. Reference [5] contains a discussion on why DASSL appears to be especially well suited for solving the TOPAZ equations.

In order for the DASSL solution to proceed, the set of TOPAZ differential and algebraic equations must be cast into the following form:

$$F [t, y(t), y'(t)] = 0 \quad (27)$$

$$y(t_o) = y_o \quad (28)$$

$$y'(t_o) = y'_o \quad (29)$$

where $y' = dy/dt$, and F , y , y' are one-dimensional vectors having a length, $I_{\max}$, the total number of equations making up the particular TOPAZ model. In the above notation F is the set of equations in residual form (all terms appearing on one side of the equals sign, see *e.g.* reference [6]), y is the vector of dependent variable values, and y' is the the vector of time derivatives of y . Equations (28) and (29) represent the initial conditions for the TOPAZ model.

In order to solve the system of equations, DASSL replaces the time derivative in (27) by a difference approximation and then solves the resulting equations at the current time, t_n , using implicit Newton iterations. Consider, for example, using a first order backward difference for y' , in which case equation (27) becomes

$$F \left(t_n, y_n, \frac{y_n - y_{n-1}}{t_n - t_{n-1}} \right) = 0 \quad (30)$$

where n represents the time step index. The system of ODE's given in (27) have, been approximated by a system of nonlinear algebraic equations (30) where y_n represents the vector of unknowns at time step n .

DASSL does not restrict itself to approximating y' using only first order approximations. Instead DASSL approximates the derivative y' using the k th order backward differentiation formula where k may range from one to five. The order k and the timestep $\Delta t_n = t_n - t_{n-1}$ is automatically chosen by DASSL at every time step based on the behavior of the solution.

The implicit iteration technique used to solve the system of nonlinear algebraic equations is Newton's method [6]. Newton's method, like any iteration scheme, requires an initial guess for the vector of unknowns. The method converges most rapidly when the initial guess is an accurate one. DASSL obtains an initial guess for y_n by evaluating the polynomial which interpolates the computed solution at the last $k + 1$ times at the current time t_n . An initial guess for y' is obtained by taking the time derivative of the interpolating polynomial and evaluating it at t_n .

DASSL provides for two options in computing the iteration matrix required in Newton's method. The user may either provide an analytic Jacobian (matrix of partial derivatives $\partial F_i / \partial y_i$) or request that DASSL compute a numerical Jacobian using finite differences. Because of the complexity of most TOPAZ models that latter option is used exclusively.

DASSL automatically selects a time increment Δt_n which satisfies a user specified set of error tolerances. The user specifies absolute and relative error tolerances either uniformly (*i.e.* one pair of tolerances for all variables) or as a vector of length $I_{\max}$ (*i.e.*, a different pair for each variable). DASSL automatically recomputes the numerical Jacobian with

varying frequency as the solution evolves. The frequency of this calculation depends on the behavior of the solution.

The DASSL user may specify a problem as having either a "banded" or "dense" variable-equation connectivity matrix. (See reference [3] for an explanation of bandedness as it applies to TOPAZ-like flow problems.) Banded problems can be solved more economically since the number of calculations required to perform the numerical differencing is substantially reduced along with the amount of computer storage.

In problems with flow branching, the banded variable-equation connectivity typified by single stream flow problems quickly breaks down. When this happens one must resort to performing DASSL calculations with a "dense" iteration matrix. TOPAZ-DASSL calculations are always performed with a dense iteration matrix.

In general the computer storage required by DASSL far exceeds the storage required by the TOPAZ code when a dense iteration matrix is used. Hence it is the storage required by DASSL which ultimately limits the size of any problem modeled by TOPAZ. Such a limitation is typical whenever equations are solved implicitly rather than explicitly. Thus far, all TOPAZ simulations to date have required substantially less than 1 M words of storage.

TOPAZ employs a special version of DASSL referred to as DASSLRT. This version of DASSL has root finding capabilities. These special capabilities are essential when flows make the transition between being choked and unchoked. Furthermore, root finding is also required for resolving several piston motion situations.

The root finding capabilities in DASSL permit the timely stopping and restarting of time integrations when certain conditions arise. For example, if the flow at a particular location is accelerated such that the local velocity approaches and then finally equals the local isentropic sound speed, this condition will be flagged by the "root finder". In this situation the root finding routines compare the calculated value of the local velocity, which is obtained from the local gas mixture momentum equation (6), to the local sonic velocity. This comparison is performed each time DASSL completes a time step. At the precise moment in time when the calculated velocity becomes equal to the local sonic velocity, the time integrations are stopped. This provides the opportunity to replace the local gas momentum equation (6) with the local sonic choking equation (22). The time integrations are then restarted and continue until another "root" is found or until the time reaches the maximum user specified problem time.

The situations in which time integrations are stopped by the root finder may be summarized as follows:

1. Transition from unchoked to choked flow.
2. Transition from choked to unchoked flow.
3. The initiation of piston motion which occurs when the piston forces exceed the

breakaway force.

4. The impact of a piston against a mechanical stop.
5. The departure of a piston from a mechanical stop.
6. A piston overcoming Coulomb friction.
7. A piston stalling (coming to rest) because of Coulomb friction.

Generally, the cost of finding roots is high (from a computational time standpoint). This is true because DASSL is forced to cut back on the time step so that integrations will stop at the precise moment in time when a root is found. Furthermore, additional computational time is required to restart the calculations. These are the primary reasons for suppressing flow choking at all locations except those coinciding with flow area expansions.

VI. AN OUTLINE OF TOPAZ CODE ARCHITECTURE

Figure 6 illustrates the major features of the TOPAZ code architecture. The figure shows the relationship between the user, the TOPAZ code, and the numerical integration code DASSL. Also shown are the functions of the various code modules.

The first step in TOPAZ simulation of gas transfer systems is the creation of an input file. This function is performed by the user according to the simple rules outlined in the TOPAZ user's manual [1]. All information required to define the user's particular problem appears in the input file, *i.e.* mesh generation information, initial conditions, requests for intermediate printouts (referred to as "edits"), and specification of $t_{\max}$, the time when calculations should be terminated.

The TOPAZ input processing routines read the user's input file line by line, checking for syntax errors. If errors are encountered, an appropriate message is printed to the user's output file and execution terminates. If the complete input file is read successfully, TOPAZ proceeds to the next step, dynamic memory allocation. Dynamic memory allocation is used to expand core memory to fit the size of the user's particular problem. This usually involves calls to machine-dependent memory expansion subroutines.

After memory expansion, mesh generation routines are used to generate the TOPAZ finite difference mesh. The code checks for user mesh generation errors and terminates with an error message if such errors are detected. Next, the code calculates the initial values for the y and y' vectors (vector of dependent variables and their time derivatives) based on the user-specified initial conditions. Included in the y vector are all the CE values for the species masses, mixture internal energy, and mixture density. These values are used to specify local thermodynamic states thus permitting the calculation of all required thermodynamic and transport properties. Gas properties are computed in the TOPAZ property routines.

With the current gas properties computed, TOPAZ is ready to advance the time step. This is accomplished by a call to DASSL. TOPAZ calculates the current values for all equation residuals (the F vector) and supplies this information to DASSL. DASSL uses this information to integrate in time over the TOPAZ-specified time interval. During this integration, DASSL selects appropriate integration time steps in order to maintain the user specified error tolerances. DASSL also checks for "roots" (see previous section) and returns control to the TOPAZ routine when appropriate (*i.e.* whenever a root is found) so that calculations may be restarted with the correct modeling equations. As indicated in Figure 6, DASSL includes LINPACK and SLATEC routines to perform the time integrations. If the time integration is performed successfully, the updated values for the y and y' vectors are returned to TOPAZ. An unsuccessful integration results in program termination and

Figure 6. TOPAZ code architecture

an appropriate error message written to the user's output file.

Upon successful integration to the new value of time, t , TOPAZ checks to see if intermediate edits (printouts to the user output file) are required. The code then checks to see if the current time is equal to the user specified termination time, $t_{\max}$. If not, TOPAZ continues to advance the time step using DASSL until $t_{\max}$ is reached. When $t_{\max}$ is reached execution is terminated.

VII. CONCLUDING REMARKS

TOPAZ (Transient One-dimensional Pipe flow AnalyZer) is a highly general user friendly computer code for modeling multi-species gas transfer through arbitrary arrangements of pipe, valves, vessels, and flow branches. Following the techniques first suggested for LOCA modeling, TOPAZ modeling utilizes the method of lines to reduce the governing one-dimensional-transient conservation PDEs to a more tractable but larger set of ODEs. An upwind, displaced mesh finite difference method is used to spacially discretize the original PDEs. Multi-dimensional flow physics is resolved through the use of quasi-steady locally-applied pressure drop and heat transfer correlations. The flow equations together with equations which describe the coupled movement of containment boundaries form the TOPAZ mathematical model. This set of mixed differential/algebraic equations is solved using the fully implicit solver DASSL (Differential/Algebraic System Solver).

This report together with references [1] and [2] represent the core documentation for the present version of the computer TOPAZ. This document is intended to acquaint potential TOPAZ users with the equations which form the TOPAZ mathematical model, the method used to solve the equations, and the overall TOPAZ code architecture. Obviously, many modeling and coding details had to be left out in order to keep this report concise. Those interested in specific details which were not discussed here are invited to consult with the author directly or to examine the TOPAZ and DASSL Fortran source codes. Each source listing contains a considerable amount of detailed information in the form of imbedded comments.

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