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MassTran (v0.19) Theory Guide

Radoslav Bozinoski

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185
Livermore, California 94550

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ABSTRACT

The purpose of this report is to document the theoretical models utilized by the computer code MassTran. This report will focus on the theoretical models used to analyze high Mach number, fully compressible, transonic flows in pipes and networks.

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1. INTRODUCTION

Navier-Stokes flow analysis of internal flow systems is usually performed on mature designs at the component level. Fine mesh resolution requirements at the component interfaces make Navier-Stokes analysis very resource intensive and possibly intractable. However, during the preliminary design phase, network flow methodologies can be used to perform analysis at the system level. The first dedicated network flow analysis tools used at Sandia were Topaz [11, 12, 13, 14, 15] and Netflow [4]. In this report, the computer code MassTran is presented. It was developed to replace Netflow and represents the third generation of network flow modeling tools.

This report will focus on the MassTran theoretical models used to analyze high Mach number fully compressible transonic flows in piping networks.

1.1. THE NEXT GENERATION ANALYSIS TOOLS AND NETFLOW

Netflow was developed as a replacement to Topaz and represents the second generation in modeling network flow problems. It has more extensive models for flow boundary conditions and gas mixture thermodynamics, improved correlations, the ability to model containment heat conduction and a slightly different, but equivalent, spatial finite difference method when modeling tubing runs. Netflow was also written as a library that can be used in other more specialized programs.

When designing the next generation tools, the use of Netflow as a library was initially considered. The following capabilities were defined as requirements for our future modeling needs:

- Ability to easily extend a component libraries and physics
- Ability to create specialized stand alone tools
- Ability to use the latest solvers

Evaluating Netflow against the above criteria highlighted certain restraints that ultimately made it unsuitable for our purposes.

The majority of Netflow is written in Fortran95 with portions in Fortran77. Its library architecture is also not general enough to be used for specialized stand alone tools. With the exception of extending constituent models, using Netflow as a library results in monolithic code development

which makes it difficult for new developer to make contributions to the code. Netflows architecture also makes extending component physics difficult[1](see figure 1-1).

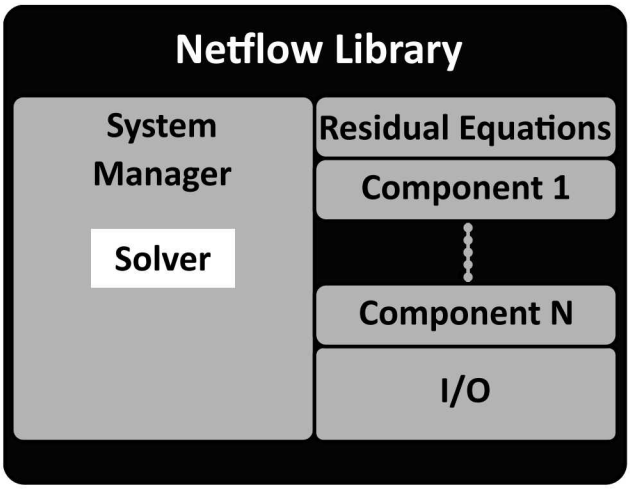


Figure 1-1. Diagram of the Netflow library architecture.

There are also difficulties in upgrading the solver used in Netflow. The system of ordinary and algebraic equations, which make up a Netflow model, are solved using the differential-algebraic system solver developed by Petzold [9]. This solver, DASKR, is no longer supported and has been replaced by IDA [6]. Much of the Netflow architecture is customized for use with DASKR and upgrading to IDA requires a major effort.

1.2. THE NEXT GENERATION ANALYSIS TOOLS AND A GENERAL FRAMEWORK

To help overcome the restraints outlined in the previous section, a new framework has been developed (see figure 1-2). The framework is written without any knowledge or assumptions about the component physics being solved and is basically a wrapper around the solver with a base component template.[2]

An example component library and analysis tool are shown in figure 1-3. Here we see how the physics defined for the component are truly modular. The analysis tool diagram also demonstrates how the framework library lends itself to the creation of specialized stand alone tools while leveraging external libraries.

[1]Referring to figure 1-1 you will notice that the residual equations module is part of the main library. What this means, in practice, is that any new components with specialized physics equations will require changes to the Netflow residual module. This negates it's usefulness as a general purpose library.

[2]In figure 1-2 we see that the component residual equations are not defined in the framework library. It is left to the developer to define the residual equations in an external component library (see figure 1-3).

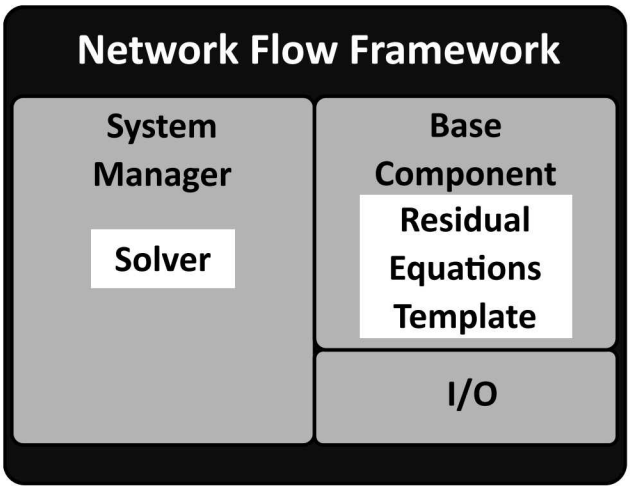


Figure 1-2. Diagram of the network flow framework architecture.

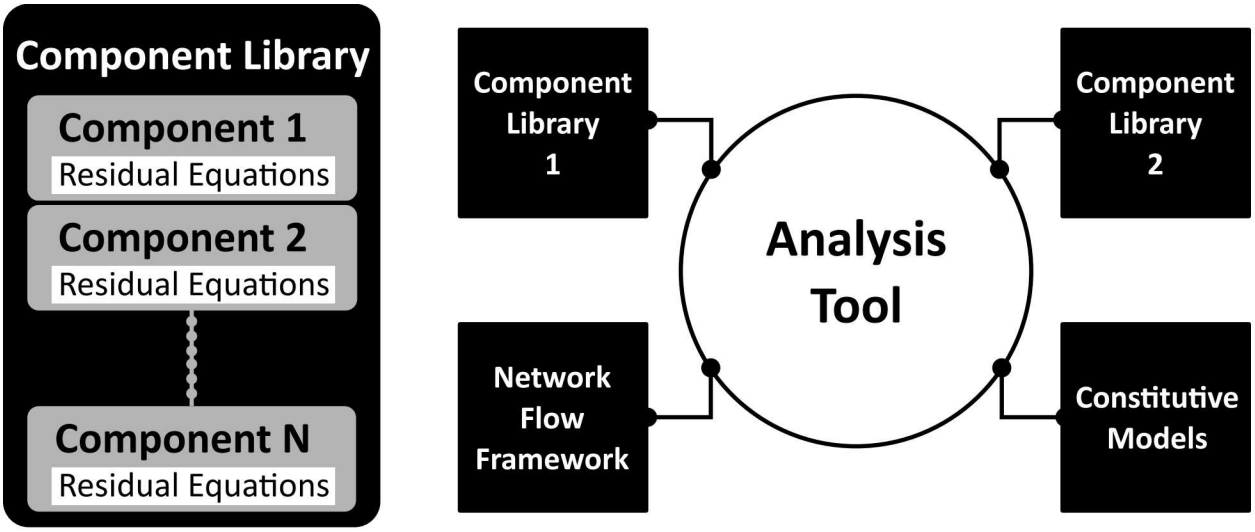
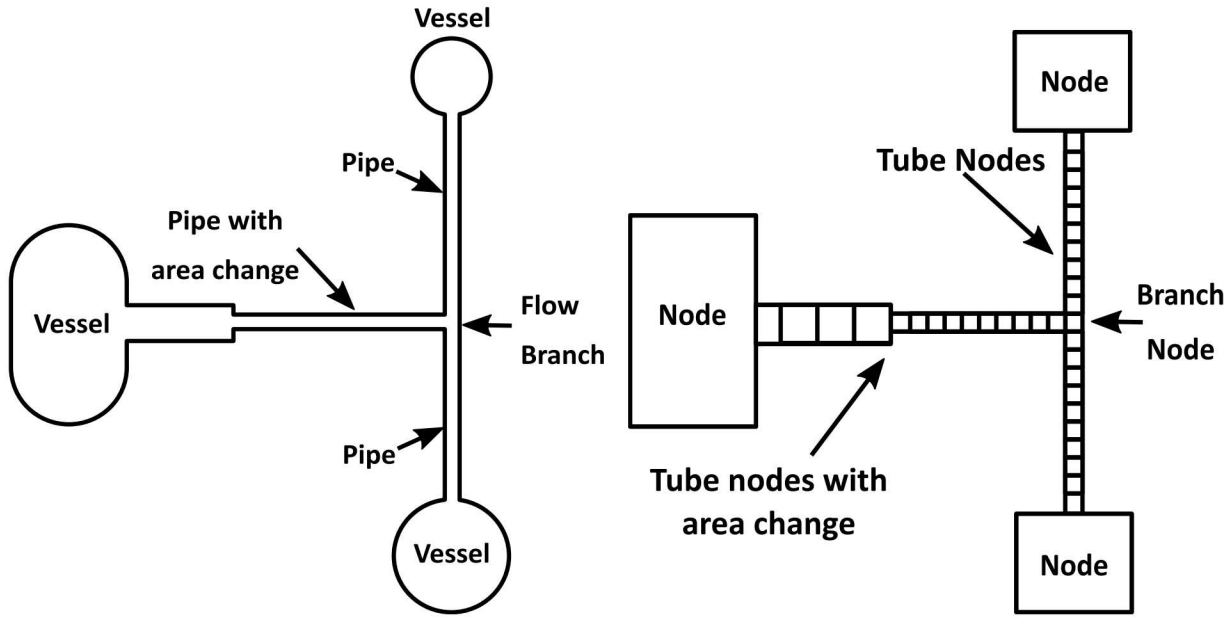


Figure 1-3. Component library and analysis tool architectures.

1.3. THE NEXT GENERATION ANALYSIS TOOLS AND MASSTRAN

Netflow's high Mach number modeling capabilities have been ported into the framework. A mass transport (MassTran) component library has been developed that enables users to model compressible flows of multi-species gas mixtures through arbitrary arrangements of pipes, vessels, and flow branches. These flow networks can be represented as a patchwork of nodes and paths (see figures 1-4(a) and 1-4(b)).

Nodes are used to simulate physical volumes in the flow network, such as pressure vessels, flow branches, and pipes. They are places in the network where scalar fluid properties are computed and conserved through the species continuity and energy equations.



(a) Example system diagram

(b) Control volume representation of system

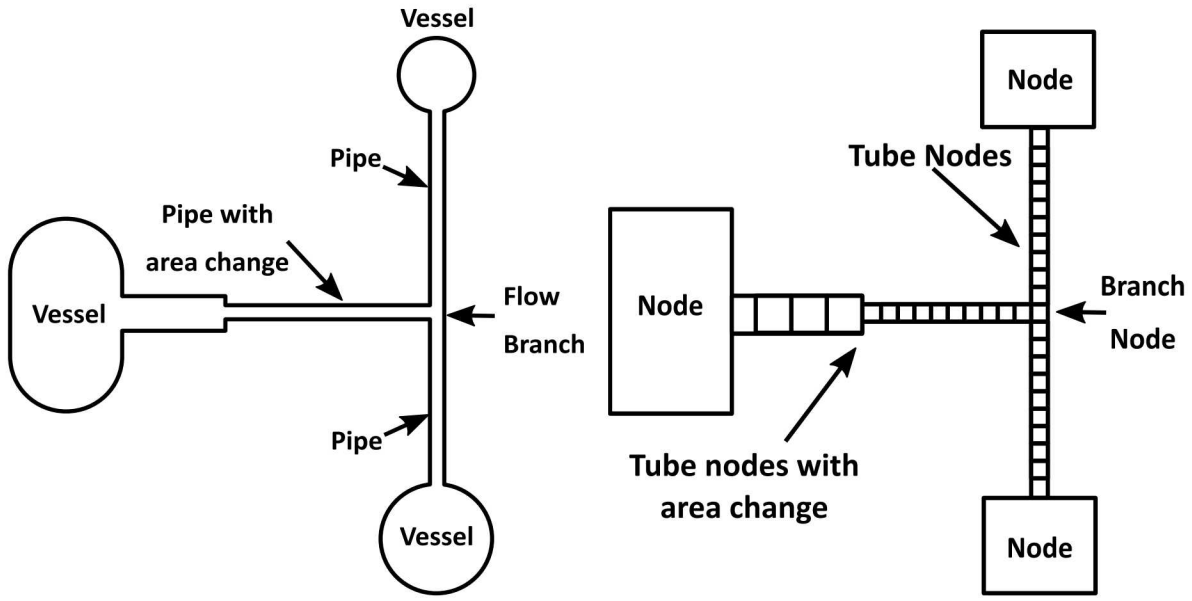
Figure 1-4. Network flow example model.

Paths are connections between nodes where fluid flow can take place. Paths have no physical volume and may be visualized as a flow interface between two nodes. They are places in the network where vector fluid properties like velocity and mass flow rate are computed and conserved according to the fluid mixture momentum equation. These properties are vector quantities since they can have both magnitude and direction (direction being either positive or negative).

2. MASSTRAN SPATIAL DISCRETIZATION

The spatial discretization used when deriving the finite difference equations for mass, energy, and momentum conservation are presented in this chapter. The method used in subdividing arbitrary fluid flow systems into finite difference networks will also be discussed.

The flow networks can be represented as a patchwork of nodes and paths (see figures 2-1(a) and 2-1(b)). In order to model this, it is necessary to discretize the network into a number of control volumes called nodes. In figure 2-1 each vessel is represented by a single node, or control volume, and each length of tubing is represented by a series of nodes. One tube is split into two made up of 4 and 10 nodes, respectively. The other two tubes are represented with 10 nodes each. Hence, for this model the network has been divided into a total of 37 nodes. They represent locations where mass of each gas species and energy of the gas mixture must be conserved. Thus, 37 gas mixture energy equations must be satisfied. The number of gas species mass conservation equations that must be satisfied is 37 times the number of species present in the gas mixture.



(a) Example system diagram

(b) Control volume representation of system

Figure 2-1. Network flow example model.

All nodes in the network model are linked to each other by flow paths. These paths are not shown in the figures but their positions align with the interfaces between the nodes. In this model, there are 36 connections between the 37 nodes. Hence, there are 36 paths in the model where the mixture momentum must be satisfied.

It is useful to think of nodes as scalar control volumes where all system scalars are computed (e.g. the density of each gas species, the mixture internal energy, pressure, enthalpy, etc.). The paths are where vector quantities, such as mass flow rate or velocity, are computed. Their directions are limited to either forward flow (a positive flow from the upstream node to the downstream node) or reverse flow (a negative flow from the downstream node to the upstream node).

In some cases it is necessary to extrapolate properties from the place where they are computed to other locations in the flow. For example, the mass flow rate for gas in a node must be extrapolated from the mass flow rates computed at connected paths. This is usually accomplished using simple averaging techniques as will be discussed later. In a similar manor, some scalar properties for paths must be extrapolated from adjacent nodes. In this case they are almost always taken from the upwind or upstream node rather than from an averaging of the upstream and downstream nodal values.

3. MASSTRAN GOVERNING EQUATIONS: NODES

The following equation types are used to build a MassTran model for a node:

1. Gas species mass conservation equations
2. Gas mixture energy conservation equations
3. The equation of state (EoS)
4. Wall heat conduction

These equation types are used to calculate the transport of a compressible gas mixtures in large tanks, flow branches, and tubes. The main differences between these components is their defined geometry and the wall heat transfer model used. At a minimum, a single gas species and energy equation are solved.

3.1. SPECIES CONTINUITY EQUATION

In general, nodes account for the transport of compressible gas mixtures. Therefore, the species continuity equations must be solved in order to track the total mass in a node as well as the individual species concentrations.

We start out with the integral form of the Species Continuity Equation:

$$0 = \frac{\partial}{\partial t}\int_{CV} \rho dV + \int_{CS} \rho \vec{v} d\vec{A} \tag{3.1}$$

where the first term represents the rate of change of mass within the control volume and the second term represents the net rate of mass flux through the control surface.

By integrating over the control volumes and surfaces we get the following macroscopic mass balance equation for node N:

$$\frac{dm_{N,k}}{dt} = -(\rho v A)_{CS} + \text{Source Terms} \tag{3.2}$$

$$\frac{dm_{N,k}}{dt} = \sum_{j=1}^{J} S_j Y_{j,k} \dot{m}_j + \dot{S}_{N,k} \tag{3.3}$$

where,

- S_j = +1 for inflow, -1 for outflow,
- $\dot{m}_j$ = mass flow through surface j [kg/s],
- $Y_{j,k}$ = mass fraction of species k at surface j
- $m_{N,k}$ = mass of species k at node N [kg],
- $\dot{S}_{N,k}$ = source term for species k at node [kg/s].

The total mass of the gas mixture in the control volume is computed as follows:

$$m_N = \sum_{k=1}^{K} m_{N_k} \tag{3.4}$$

3.2. MIXTURE ENERGY CONSERVATION

The mixture energy conservation for the nodal control volume is a simple statement of the First Law of Thermodynamics:

> The time rate of change of energy within the node is equal to sum of the incoming energy flow rates minus the outgoing energy flow rates plus the heat transferred from the containment walls plus any internal energy generated (or removed) from the control volume .

To derive the energy relationship for the control volumes we can start with the first law of thermodynamics and get the following integral form of the equation:

$$\dot{Q} - \dot{W} = \frac{\partial}{\partial t} \int_{CV} e\rho dV + \int_{CS} e\rho \vec{v} d\vec{A} \tag{3.5}$$

By integrating over the control volumes and surfaces we get the following form:

$$\dot{Q} - \dot{W} = \frac{dE_{CV}}{dt} - \sum_{CS} e\dot{m} = \frac{dE_{CV}}{dt} - \sum_{CS} \dot{m} \left(u + \frac{v^2}{2} + gz \right) \tag{3.6}$$

The energy transfer from work can be split up into pressure work and all other control volume work.

$$\dot{W} = \dot{W}_{CV} + \sum_{CS} \dot{m} \frac{P}{\rho} \tag{3.7}$$

Moving the above into the energy equation and rearranging we get the following:

$$\frac{dE_N}{dt} = \dot{Q}_N - \dot{W}_N + \sum_{j=1}^{J} S_j \dot{m}_j \left(h + \frac{v^2}{2} \right)_j \tag{3.8}$$

where,

- S_j = +1 for inflow, -1 for outflow,
- $\dot{m}_j$ = mass flow through surface j [kg/s],
- $\dot{Q}_N$ = the net rate of energy transfer by heat across the control volume boundary for node N [J/s],
- $\dot{W}_N$ = the net rate of energy transfer by work across the control volume boundary for node N [J/s],
- $h = u + \frac{P}{\rho}$ = the gas mixture specific enthalpy [J/kg],
- $E_N = m_N(u_N + \frac{v_N^2}{2})$ = the total energy of the control volume for node N [J].

The node control volume velocity, v_N, is calculated from the following expression:

$$v_N = \frac{\dot{m}_N}{A_N \rho_N} \tag{3.9}$$

where,

- $\dot{m}$ is the control volume mass flow rate at node N [kg/s],
- A_N is the control volume cross-sectional area for node N [m^2],
- ρ_N is the control volume density for node N [kg/m^3].

The control volume mass flow rate must be interpolated from the incoming and outgoing path mass flow rates as follows:

$$\dot{m}_N = \frac{1}{2} \left(\sum_{in} \dot{m}_j - \sum_{out} \dot{m}_j \right) \tag{3.10}$$

3.3. THERMODYNAMIC AND PROPERTY RELATIONSHIPS

The flow conservation equations described in the previous sections are used to determine the mass of each species, m_{N_k}, and the internal energy of the mixture, u_N, at all nodes. Having computed two independent thermodynamic properties, namely density and internal energy, the state of the fluid is completely specified. The remaining properties required in the control volume can then be calculated directly from the known state and property relations. The relationships required for the fluid model can then be summarized as follows:

$$\begin{aligned}
\text{Pressure } P &= f_1(\rho, u, Y_1 \cdots Y_k) \\
\text{Temperature } T &= f_2(\rho, u, Y_1 \cdots Y_k) \\
\text{Enthalpy } h &= f_3(\rho, u, Y_1 \cdots Y_k) \\
\text{Specific heats } c_v &= f_4(\rho, u, Y_1 \cdots Y_k) \\
c_p &= f_5(\rho, u, Y_1 \cdots Y_k) \\
\text{Thermal conductivity } k &= f_6(\rho, u, Y_1 \cdots Y_k) \\
\text{Viscosity } \mu &= f_8(\rho, u, Y_1 \cdots Y_k) \\
\text{Isentropic sound speed } c_s &= f_7(\rho, u, Y_1 \cdots Y_k) \\
\text{Isobaric expansion coefficient } \beta &= f_9(\rho, u, Y_1 \cdots Y_k)
\end{aligned} \tag{3.11}$$

3.4. CONSTITUENT MODELS

Below are the constituent models used in MassTran node components.

3.4.1. Meyer Wall Heat Transfer Model

To solve for $\dot{Q}_N$ in equation 3.8, we can use the following heat transfer model for the net rate of energy transfer between the node gas and the container wall:

$$\begin{aligned}
\dot{Q}_N &= hA_{surf}\left(T_{wall} - T_N\right) \\
h &= \frac{kNu}{d}
\end{aligned} \tag{3.12}$$

where,

- A_{surf} = Surface area,
- Nu = Nusselt number,
- d = hydraulic diameter,

- T_{wall} = container wall temperature,
- T_N = Node temperature

For free convection, the Nusselt number can be calculated using a modified form of the Meyer correlation[16]. This model is most appropriate for a vessel acting as a source tank undergoing a monotonic pressure decay as it empty. In this case, the Nusselt number is determined from the maximum of the laminar and turbulent Nusselt numbers, i.e.,

$$\begin{aligned} Nu_{lam} &= 0.8331\, Ra^{1/4} \\ Nu_{turb} &= 0.168\, Ra^{1/3} \\ Nu_{free} &= \max(Nu_{lam}, Nu_{turb}) \end{aligned} \tag{3.13}$$

The parameter Ra in equation 3.13 is the Rayleigh number which is the product of the Grashof, Gr, and Prandtl, Pr, numbers and takes the following form:

$$Ra = GrPr = \frac{g\beta(T - T_{wall})\rho^2 d^3}{\mu^2}\frac{c_p \mu}{k} \tag{3.14}$$

where g is the gravitational constant, β is the isobaric expansion coefficient, and d is the diameter of the spherical vessel.

The numerical coefficients and exponents appearing in the free convection vessel heat transfer model (equation 3.13) were determined from experiment[17, 16]. In the experiments, all source pressure vessels where oriented so that flows exited from the bottom and all sink pressure vessels were oriented so the incoming flows entered at the top. Subsequent experiments have shown that heat transfer predictions are less accurate for other orientations.

3.4.2. Combined Wall Heat Transfer Model

The combined free and forced convection vessel heat transfer model is suggested for nodes that act as sink tanks[1]. The combined model computes a forced convection Nusselt number based on the Reynolds number of the incoming flow stream. If there are more than one incoming flow streams, Nusselt numbers for all the streams are calculated and the largest one is used. The forced convection Nussselt number for an incoming flow is computed from an equation first suggested by Means and Ulrich [8]. The model is as follows:

[1]The free convection Nusselt number is that calculated using equation 3.13

$$
\begin{aligned}
Nu_{forced_j} &= 6.694 \left[Re\, Pr \left(\frac{d}{D} \right)^2 \right]_j^{0.632} \\
Nu_{forced} &= \max(Nu_{forced_1}, ..., Nu_{forced_J}) \\
Nu &= \max(Nu_{free}, Nu_{forced})
\end{aligned}
\tag{3.15}
$$

where the Reynolds and Prandtl number are computed from the incoming flow, d is the incoming flow diameter and D is the characteristic dimension of the vessel. The forced convection Nusselt number attempts to account for the heat transfer effect of the incoming jet flow (usually supersonic) which may penetrate far into a filling vessel and contact the opposite wall. The combined model calculates a free convection Nusselt number using Equation 3.13 and a forced convection Nusselt number using Equation 3.15 and uses the largest of the two as the combined vessel Nusselt number.

It should be noted that heat transfer in a tank acting as a sink is very complicated. The influence of one or more incoming jets together with large natural convection effects later in the filling process make it difficult to characterize the heat transfer using the simple correlations presented here. For sink tanks, the user should expect that the combined model is only an approximation. References [17] and [16] demonstrate the accuracy one can expect under the best of circumstances.

3.4.3. Dittus-Boelter Wall Heat Transfer Model

For tube or pipes, the turbulent wall heat transfer model based on Dittus-Boelter[7] should be used. The heat transfer is applied to the path surface areas of the attached upstream and downstream nodes. As is the case for friction factors, tube flow forced convection heat transfer models apply to fully developed flow and must only be regarded as approximations for developing flow regions. The turbulent Nusselt number is based on the correlation developed by Dittus and Boelter is as follows:

$$
\begin{aligned}
Nu_{lam} &= 4.364 \\
Nu_{turb} &= 0.23\, Re^{0.8}\, Pr^{0.4} \\
Nu &= \max(Nu_{lam}, Nu_{turb})
\end{aligned}
\tag{3.16}
$$

4. MASSTRAN GOVERNING EQUATIONS: PATHS

The following equation types are used to build a MassTran model for a path:

1. Gas mixture momentum conservation equations
2. Constituent flow loss models

4.1. MIXTURE MOMENTUM BALANCE

The momentum equation for a path is a straightforward application of Newton's second law which states that:

> The sum of all forces (surface and body forces) acting on a non-accelerating control volume is equal to the sum of the rate of change of momentum inside the control volume and the net rate of flux of momentum out through the control volume.

To derive the mixture momentum balance we start with Newton's second law and get the following integral form of the vector equation:

$$\vec{F} = \vec{F}_S + \vec{F}_B = \frac{\partial}{\partial t}\int_{CV} \vec{v}\rho dV + \int_{CS} \vec{v}\rho\vec{v}d\vec{A} \tag{4.1}$$

In the above, the surface forces acting on the control volume can be broken into those due to pressure and those due to losses:

$$\vec{F}_S = -\int_{CS} Pd\vec{A} - losses \tag{4.2}$$

In general, the effects of losses are to decrease the pressure and can be divided into major (due to friction in constant-area portions of the system and flow through porous media) and minor[1] (due to flow through valves, tees, and elbows) contributions.

The pressure force term can be further simplified as follows:

[1] In general minor losses and body forces are neglected.

$$-\int_{CS} P d\vec{A} = A_j \left(P_{N,up} - P_{N,dn}\right) \tag{4.3}$$

The momentum flux term on the right hand side (RHS) of 4.1 can also be simplified by integrating over the control surfaces to get the following:

$$\int_{CS} \vec{v}\rho\vec{v} d\vec{A} = -A_j \left([\rho v^2]_{N,up} - [\rho v^2]_{N,dn}\right) \tag{4.4}$$

By integrating the rate of change of momentum inside the control volume on the RHS of 4.1 and substituting 4.2, 4.3, and 4.4 the macroscopic form of the momentum balance equation:

$$A_j \left(P_{N,up} - P_{N,dn}\right) - losses = \frac{d}{dt}\left(\rho v V\right)_N - A_j \left([\rho v^2]_{N,up} - [\rho v^2]_{N,dn}\right) \tag{4.5}$$

The rate term in the above equation can further be simplified as follows:

$$\rho v V = L\dot{m} \tag{4.6}$$

Using the above simplification and further rearranging, the final form of the macroscopic mixture momentum balance equation is:

$$I_j \frac{d\dot{m}_j}{dt} = \left(P_{N,up} - P_{N,dn}\right) + \left([\rho v^2]_{N,up} - [\rho v^2]_{N,dn}\right) - losses \tag{4.7}$$

where,

- I_j = the geometric inertia term [m^{-1}],
- $\rho_{N,up}$ = the density of the gas mixture in the upstream node [kg/m^3],
- $\rho_{N,dn}$ = the density of the gas mixture in the downstream node [kg/m^3],
- $v_{N,up}$ = the velocity of the gas mixture in the upstream node [m/s],
- $v_{N,dn}$ = the velocity of the gas mixture in the downstream node [m/s],
- $P_{N,up}$ = the pressure of the gas mixture in the upstream node [Pa],
- $P_{N,dn}$ = the pressure of the gas mixture in the downstream node [Pa],
- $losses$ = losses resulting in pressure drop [Pa].

The geometric inertia term is determined from the adjacent nodal control volumes and is calculated as follows:

$$I_j = \frac{1}{2}\left(\frac{L_{N,up}}{A_{N,up}} + \frac{L_{N,dn}}{A_{N,dn}}\right) \tag{4.8}$$

where L is the node length and A is the node cross-sectional area.

4.2. CONSTITUENT LOSS MODELS

The models that follow present loss coefficients that are used for equation 4.7 in the following form:

$$losses = \Delta P = \frac{1}{2} K \rho \vec{v} |\vec{v}| \tag{4.9}$$

4.2.1. Pipe Friction

A Pipe friction loss coefficient can be obtained for equation 4.9 using a single correlation model defined by Churchill[5]. The model is presented below as the commonly used Darcy friction factor[2].

$$\begin{aligned} f &= 8\left[\left(\frac{8}{Re}\right)^{12} + \frac{1}{(A+B)^{3/2}}\right]^{1/12} \\ A &= 2.457\, ln\left(\frac{1}{\frac{0.27\varepsilon}{d} + \left(\frac{7}{Re}\right)^{0.9}}\right)^{16} \\ B &= \left(\frac{37{,}530}{Re}\right)^{16} \\ K_{fric} &= \frac{fL}{d} \end{aligned} \tag{4.10}$$

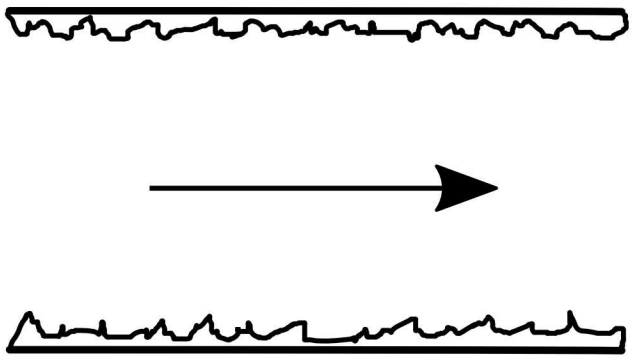


Figure 4-1. Diagram of the pipe friction loss.

[2]For Re below 1, the friction factor is set to 64. This was done because numerical stability issues arise as Re goes to zero

4.2.2. Area Change

The area loss coefficient[2] due to flow expansion and contraction is defined as follows:

$$K_{contraction} = \frac{1}{2}\left[1 - \frac{A_2}{A_1}\right]$$
$$K_{expansion} = \left[1 - \frac{A_1}{A_2}\right]^2 \tag{4.11}$$

where,

- A_1 = Upstream tube area,
- A_2 = Downstream tube area.

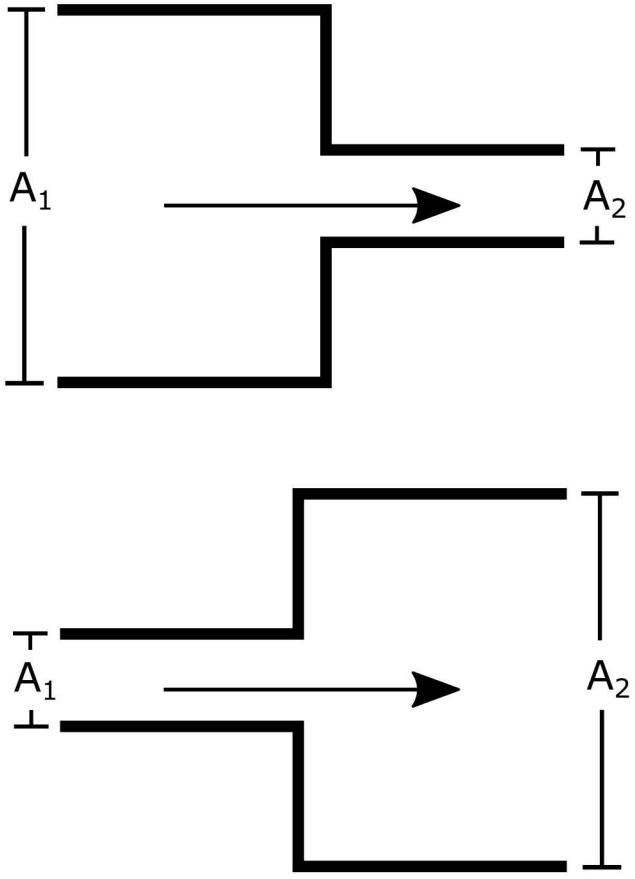


Figure 4-2. Diagram of area change losses.

4.2.3. Porous Media Filter

Pressure loss through a porous media filter is calculated using a form of the dusty gas model developed by Shugard[10] and is as follows:

$$
\begin{aligned}
losses &= \frac{\dot{m}\bar{R}TL}{MWA\left(D^K + \frac{B}{\mu}\bar{P}\right)} \\
D^K &= \frac{4}{3}K_o\sqrt{\frac{8\bar{R}T}{\pi MW}} \\
\bar{P} &= \frac{1}{2}\left(P_{up} + P_{dn}\right)
\end{aligned}
\tag{4.12}
$$

where,

- D_K = Knudsen diffusion,
- K_o = Molecular flow coefficient,
- B = Permeability.

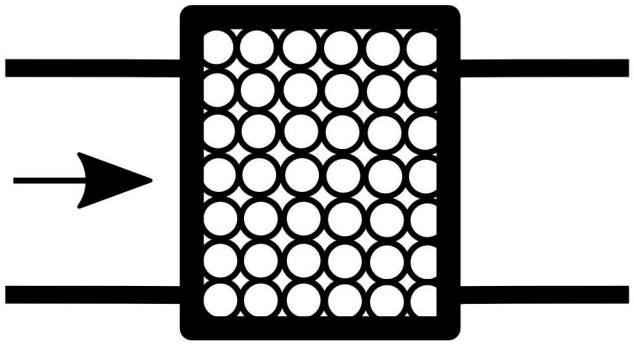


Figure 4-3. Diagram of porous media filter loss.

When using this model an experimentally obtained constant, K_o, must be supplied by the user.

4.2.4. Valve

For those cases when a flow path is used to simulate a valve that has been experimentally characterized using flow rate and pressure drop data, the valve flow model developed by Bozinoski al el.[3] may be used. The model accounts for both choked and unchoked flow through the valve. Three experimentally obtained constants, a, b, and ψ_{crit} must be supplied by the user. Valve losses for subsonic flow are calculated as follows:

$$\begin{aligned} \psi &= \frac{\dot{m} c_s}{P_{up} A}; \quad \phi = \psi^2 \\ \beta &= \frac{\Delta P}{P_{up}} = a\phi^2 + b\phi \\ losses &= S\beta P_{up} \end{aligned} \tag{4.13}$$

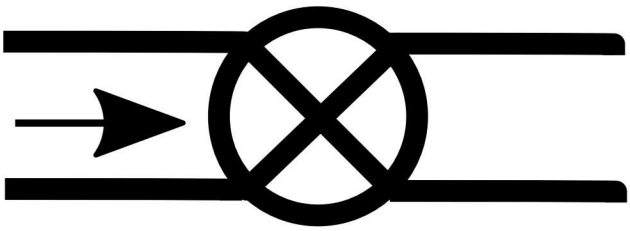


Figure 4-4. Diagram of valve.

where,

- S = +1 for inflow, -1 for outflow,
- ψ = Flow factor,
- β = Non-dimensional pressure,
- c_s = Fluid sound speed,
- a, b = Empirical coefficients.

When $\psi > \psi_{crit}$ we have choked flow and the following algebraic model is used to calculate the mass flow rate:

$$\dot{m}_{crit} = \frac{A P_{up} \psi_{crit}}{c_s} \tag{4.14}$$

where,

- ψ_{crit} = Critical flow factor,
- $\dot{m}_{crit}$ = Critical mass flow rate.

4.2.5. Orifice

Orifice losses[2] for subsonic flow are calculated as follows:

$$
\begin{aligned}
losses &= \frac{8}{\rho}\left(\frac{\dot{m}}{\pi d^2 c_d Y}\right)^2\left[1-\left(\frac{d}{D}\right)^4\right] \\
Y &= 1-\left[0.41+0.35\left(\frac{d}{D}\right)^4\right]\frac{P_{up}-P_{dn}}{\gamma P_{up}}
\end{aligned}
\tag{4.15}
$$

where,

- d = Orifice diameter,
- D = Upstream tube diameter,
- c_d = Loss coefficient,
- Y = Expansion factor,
- γ = Specific heat ratio.

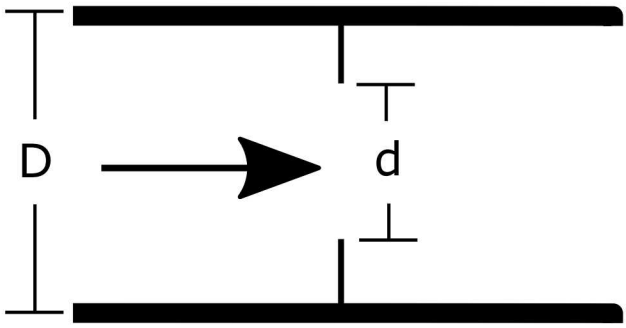


Figure 4-5. Diagram of thin, sharp orifice.

4.3. ISENTROPIC FLOW MODEL

The equations presented in the previous sections represent the most often used relationships for describing flows in paths. The accuracy of these equations is heavily dependent on our ability to characterize the form loss coefficients, however. These form losses are intended to account for all wall friction and multidimensional flow effects not directly modeled by the one-dimensional flow momentum equation(4.7). Often these form losses are unknown or not adequately represented. We know, for example, that the area change form loss expressions defined in section 4.2.2 are intended for incompressible flow in which the local Mach number is less than approximately 0.3. What if the local Mach number is 0.9? Similarly, we know that characterizing the frictional

pressure loss using the equations presented in section 4.2.1 are adequate for quasi-steady fully developed flow in a straight tube. What if the flow is not fully developed or the tube is not straight?[3] In these cases the models must be regarded as approximations.

In some cases, the previously described flow losses may be less accurate than just assuming isentropic flow through the path. This is sometimes true for the case where flow is being accelerated from stagnation conditions in a source tank to high speed flow in the exit tubing. The previously described finite difference models may be less accurate than assuming isentropic flow [4][4].

For these reasons, an isentropic flow path model is provided that can be used to define the flow physics in a path. This model is identical to that outlined by Bird, Stewart and Lightfoot[1] for flow of an ideal gas.

4.4. CHOKED FLOW ALGORITHM

In quasi-steady compressible flow, the flow at area expansions can become choked. A choked flow occurs when the pressure downstream of the choke point becomes so low that the flow speed at the choke point reaches the sonic velocity. Downstream of this location the flow becomes supersonic until a series of shock waves restores the flow to subsonic conditions. The one-dimensional mixture momentum equation(4.7) cannot be used to describe choked flow since downstream pressure signals cannot propagate upstream to impact the flow rate. Saying it another way, the flow at the choke point has no knowledge of the pressure downstream and as result is unaffected by this pressure unless forces driving the flow cause the flow to decelerate. When the flow decelerates, the velocity at the choke point drops below it sonic value and equation 4.7 can once again be used to describe the flow rate.

In order to understand how MassTran deals with choked flow, it is useful to rewrite equation 4.7 in the following form,

$$I_j \frac{d\dot{m}_j}{dt} = RHS \tag{4.16}$$

where "RHS" are the terms on the Right Hand Side of equation 4.7. If we think of equation 4.7 as an expression of Newton's Second Law as applied to a fluid (which it is), it is easy to see that when RHS is positive the flow is accelerating and when RHS is negative the flow is decelerating. We can use this knowledge to establish the rules for describing choked and unchoked flow in MassTran. For unchoked flow, where $\dot{m}_j$ is less than the sonic flow rate, equation 4.7 is used to determine the path flow rate. Because of our upwinding of scalar properties at path locations, the sonic flow rate for a path is described by,

$$\dot{m}_{j_{sonic}} = \rho_{N_{up}} A_j c_{s_{up}} \tag{4.17}$$

[3]It often takes more than 50 tube diameters of flow at the entrance of the tube before the flow is fully developed.
[4]See Appendix B of the Netflow theory manual for a more detailed discussion

where $c_{s_{up}}$ is the speed of sound in the gas mixture at the upstream node. The speed of sound is a thermodynamic property that is determined from the equation of state for the mixture.

When the flow is choked, equation 4.17 is used to determine the path flow rate. Equation 4.17 will continue to be used to describe the path flow rate until RHS changes sign signaling a deceleration of flow below $\dot{m}_{j_{sonic}}$. Hence we can summarize choking and unchoking rules for a potential choking path (i.e.a path where the flow expands) using the following statement:

> Equation 4.7 is used until $\dot{m}_j = \dot{m}_{j_{sonic}}$, then 4.17 is used until RHS changes sign.

It can be shown that MassTran properly chokes and unchokes the flow at appropriate upstream/downstream pressure ratios. The actual region of supersonic flow and shock structure downstream of the choke are not being modeled but the proper flow rates for unchoked and choked flow are preserved.

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