

# A Transient Flow Model of Compressible Gas Mixtures in a Nuclear Fuel Processing Plant

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## ABSTRACT

A model was developed to predict mixture concentration profiles in a subatmospheric mixture of hydrogen, nitrogen, and oxygen during valve-switching between a process line and an atmospheric vent line. The switching event allows air in-leakage to the system during the period in which the routing valves are open. Hydrogen and oxygen concentrations must be predicted to assess the potential for developing combustible mixtures in the system.

The model consists of a one-dimensional finite-difference representation of the transient momentum and mass conservation equations, associated constitutive relationships and an equation-of-state for compressible gas. The resulting equation set was solved with Advanced Continuous Simulation Language (ACSL).

## INTRODUCTION

Oxygen leakage and the attendant potential for hydrogen detonation prompted interest in having the capability to analyze the flow and gas mixture behavior of sections of a process system. A suitable model should provide the capability to compute flow rates, pressures, gas compositions, and related variables. It should also be useful in performing parametric studies and predicting the behavior of potential system modifications.

## THEORY AND EQUATIONS

Transient flow modeling is accomplished by solving a system of simultaneous mass and

momentum conservation equations coupled with an equation of state. All but the most trivial problems require a numerical formulation executed by a computer solution. The Advanced Continuous Simulation Language (Mitchell and Gauthier 1986) provided the medium for formulating and solving the necessary mathematical relationships.

The modeling effort requires selection of an appropriate set of conservation equations and associated constitutive relationships, i.e., friction factor and heat transfer correlations (if needed) and coding them in the format required by ACSL.

The mass and momentum conservation is defined for this model in terms of one-dimensional compressible flow in finite-difference form (terms accounting for elevation head have been neglected). Spatial variation of each state variable is achieved by defining control volumes which represent the system's physical flow path. This construct is illustrated in Figure 1. The mass flow rates computed by the momentum equation apply to the junctions between control volumes. Each mass balance is associated with a region corresponding to a control volume.

Mass continuity for each gas component (hydrogen, oxygen and nitrogen) is defined as:

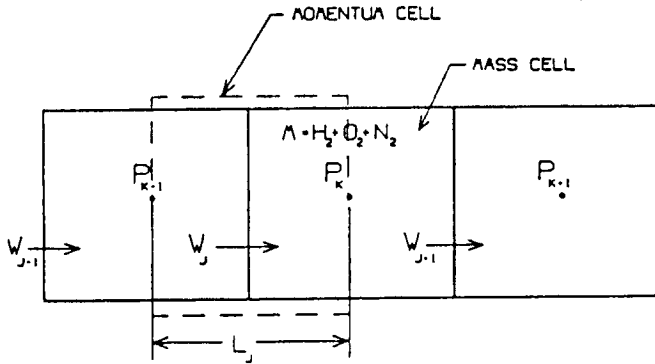
$$\frac{dM_{i,k}}{dt} = X_{i,k-1} W_j - X_{i,k} W_{j+1} \quad (1)$$

$$\text{where } X_{i,k} = \frac{M_{i,k}}{M} \quad (2)$$

$$\text{and } M = \sum M_i \quad (3)$$

This representation applies for the case of positive flow at both cell boundaries. In general, the mass fraction used in the mass balance equation must correspond to that of the donor

cell. Thus, in coding this equation, it is necessary to invoke a test on flow direction to determine the location of the donor cell.



UNIT CELL DEFINITION

Figure 1.

The molar composition is computed by an appropriate conversion of the component mass inventories:

$$MOLE_i = \frac{M_i}{m_i} \quad (4)$$

$$MOLE = \sum MOLE_i \quad (5)$$

which yields the mole fraction for each component (hydrogen, oxygen, and nitrogen) as

$$XMOLE_i = \frac{MOLE_i}{MOLE} \quad (6)$$

Mass flow rate is computed by the momentum conservation equation as follows:

$$ACCELERATION = MOMENTUM FLUX + PRESSURE DROP - FRICTION \quad (7)$$

$$ACCELERATION = \left( \frac{L_j}{A_j} \right) \frac{dW_j}{dt} \quad (8)$$

$$PRESSURE DROP = P_{k-1} - P_k \quad (9)$$

$$MOMENTUM FLUX = \left( \frac{W_v^2}{\rho A^2} \right)_{k-1} - \left( \frac{W_v^2}{\rho A^2} \right)_k \quad (10)$$

where the volume average mass flow,

$$W_{v,k} = \frac{(W_j + W_{j+1})}{2} \quad (11)$$

$$FRICTION = \left( \frac{fL}{D} + K \right) \frac{W_j |W_j|}{(2\rho_j A_j^2)} \quad (12)$$

The mass and momentum continuity equations are coupled by an equation-of-state which, using the perfect gas relationship, is

$$P_k = MOLES_k \frac{RT_k}{V_k} \quad (13)$$

$$\text{and density is } \rho_k = \frac{M_k}{V_k} \quad (14)$$

The friction factor is represented by the following simplified form:

$$f = 64/Re \text{ for } Re \leq 4000 \text{ (laminar flow)} \quad (15)$$

$$f = 0.016 \text{ for } Re > 4000 \text{ (turbulent flow)} \quad (16)$$

$$\text{where } Re = \frac{WD}{A\mu}. \quad (17)$$

The mass and flow rate derivatives are integrated within numerical integration algorithms provided by ACSL. Several integration schemes are available as options in ACSL. For this application, the variable time-step options proved to be the most efficient.

## VALVE MODEL

Describing valve behavior is a critical element of this problem. The form loss applied to frictional pressure drop is a conventional way to portray flow in a valve. The coefficient,  $K$ , in the frictional pressure drop expression represents the valve loss-coefficient. during the act of opening or closing the valve flow area varies between zero and its full-open value. In the model, the valve flow rate may be modulated simply by varying the flow area, which appears in denominator of the frictional pressure drop term. However, when the area is close to zero certain problems are encountered in the model solution.

First, the value of the area cannot be allowed to equal zero because of its position in a denominator. This problem can be avoided by constraining its minimum value to a very small number, e.g.  $10^{-5}$ . The second, more difficult problem is that very small values of this area introduce large eigenvalues into the equation set, which in turn impose small time advancements on the numerical solution. If these become small enough the problem will fail. No simple resolution of this problem was found during the course of the model development, so a constraint was placed on the derivative of the flow rate that provided a practical resolution to the problem.

During the beginning of opening or the ending of closing, the flow derivative at the valve was set to zero whenever the values of both area and flow were less than  $10^{-5}$ . This addition to the model permits the computations to proceed successfully through these events.

## MODEL VALIDATION

The conservation equations and their coding were verified by comparison with a known analytical solution for a simple problem. This consisted of the flow response to a constant pressure drop across a single control volume. The analytical formulation is:

$$\frac{d\hat{G}}{d\tau} + \hat{G}^2 = 1 \quad (18)$$

where the mass flux,  $\hat{G} = G/G_{ss}$ .

This has the solution

$$\hat{G} = \frac{G_0 + \tanh(\tau)}{1 + G_0 \tanh(\tau)} \quad (19)$$

where  $\tau$  is the time constant determined by the problem parameters. Good agreement was obtained between the analytical solution and the model equations using identical parameters in both computations.

## GAS LINE MODEL DESCRIPTION

The model represents the system configuration providing information about the potential causes of hydrogen explosion and establishes a performance baseline for future changes. It describes flow pressure and concentration profile for the piping approaching the main stack vent junction and branch lines.

The nodalization diagram of the model is shown in Figure 2. The supply line enters a branch where a pair of valves direct the flow of hydrogen either to the vent or to the process system.

The mathematical model for this configuration contains 54 state variables, i.e., variables defined by differential equations. There are 15 mass flow rates and 39 mass balances (three for each volume cell). ACSL's integrations algorithm must solve these 54 equations simultaneously.

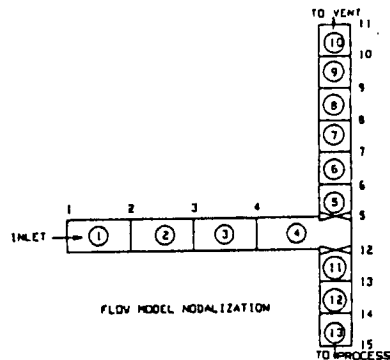


Figure 2.

Boundary conditions for the model consist of specified values of variables at the following locations:

1. Mass flow rate and gas composition at the inlet of the supply line,
2. Pressure and gas composition at the vent and process system boundaries.

The valve areas were treated as as explicit functions of time. They varied from open to closed positions or vice-versa in a specified time interval.

## ANALYSIS

The transient flow model described above was used to calculate flow rates and gas compositions for conditions corresponding to rerouting of the flow stream from vent to process system and vice-versa. During such switching air enters the system because of the pressure drop between the vent and process system. Oxygen and hydrogen mixture concentrations which result from the in-leakage of air determine the conditions for potential combustion.

In the case to be discussed, the initial flow path is established from the inlet pipe through the fully-open vent-side valve to the vent system. The vent on the process system side is initially fully closed. After flow is established (one second into the calculation) the vent valve begins to close and the process system valve begins to open. The valve travel time is two seconds.

As the process system-side valve opens the flow path will shift to this branch, since it is at the lowest pressure. Flow will reverse in the vent-side branch and then decline to zero as the vent-side valve closes.

The performance of selected variables is presented in Figures 3 through 8 which include the results of four different runs showing the influence of process system pressure. Hydrogen and oxygen concentrations at process system are shown in Figure 3.

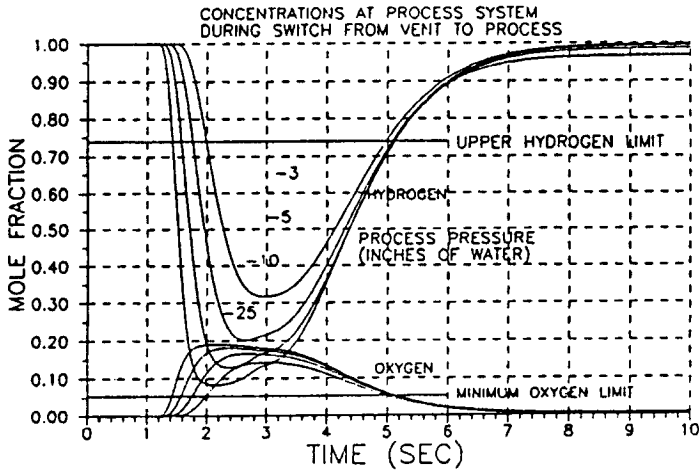


Figure 3.

As expected, in-leakage of air increases as process system pressure decreases. Mass flow rates at the process system and vent valves, respectively, are shown in Figures 4, and 5.

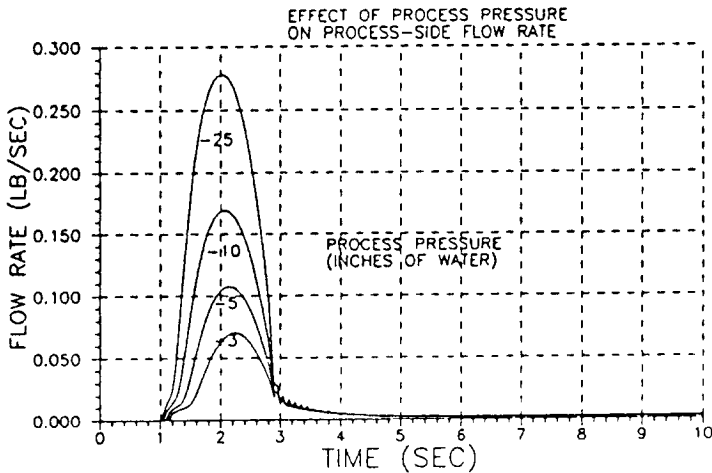


Figure 4.

The peak values of mass flow are large compared to the hydrogen flow rate because of the large ratio between the densities of hydrogen and air.

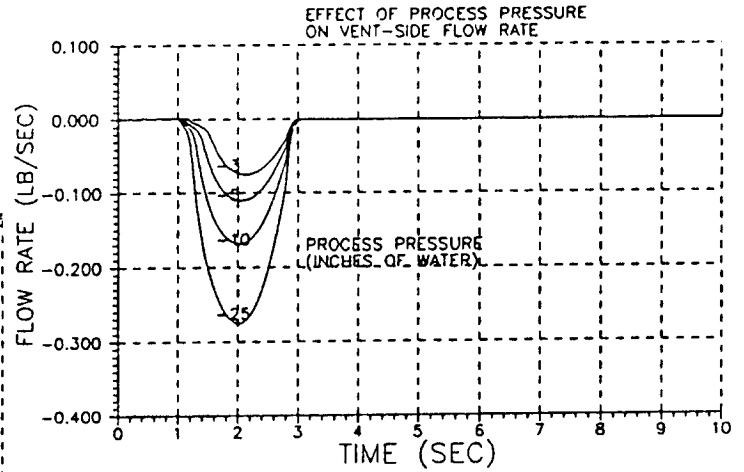


Figure 5.

Another perspective on the flows is provided by examining velocities. These are given in Figures 6, and 7 for the case having -25 inches of water in process system (the family of curves for the other pressures contain excessive overlap for clear presentation).

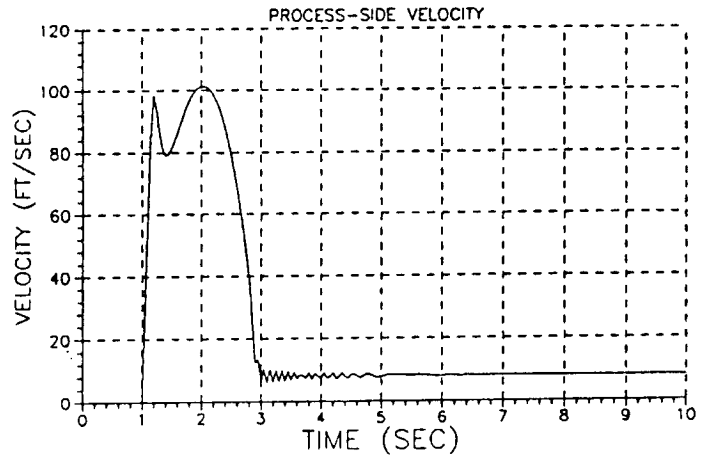


Figure 6.

The large peak velocities (100 to 150 ft/sec) reflect the effect of the sudden pressure drop change brought about by the valve opening.

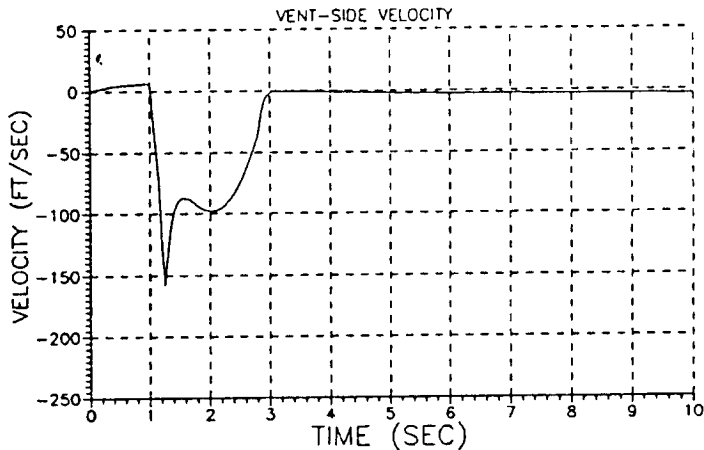


Figure 7.

Figure 8 shows the system pressure response. The transition of flow routing from vent to process system causes the pressure at the tee to traverse through values reflecting those of the two boundaries.

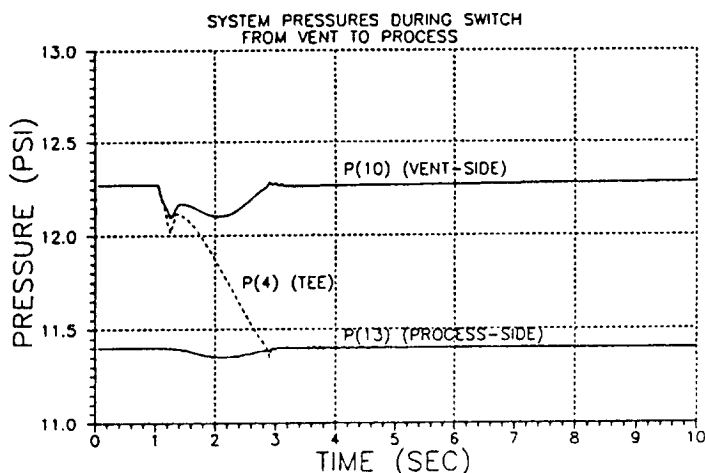


Figure 8.

The most significant product of this analysis is the range of conditions that can produce a flammable mixture of hydrogen and oxygen in the system. Figure 3 shows that a flammable mixture exists (flammable concentration limits (Haroldsen 1987) are shown on the figure) over intervals of two to three seconds for the full range of process system pressures investigated. The trends contained in the figure indicate that flammable mixtures might even be produced at process system pressures as low as one inch of

water. There is, therefore, a significant potential for hydrogen combustion during valve switching for this system configuration.

#### ACKNOWLEDGEMENT

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#### REFERENCES

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#### NOMENCLATURE

- A - Flow Area
- D - Diameter
- f - Friction Factor
- G - Mass Velocity
- K - Loss Coefficient
- L - Length
- M - Mass
- MOLES - Number of Moles
- m - Molecular Weight
- l - Viscosity
- P - Pressure
- R - Universal Gas Constant
- q - Density
- Re - Reynolds Number
- T - Temperature
- t - Time
- s - Time Constant
- V - Volume
- W - Mass Flow Rate
- $W_v$  - Volume Average Mass Flow Rate
- XMOLE - Mole Fraction
- x - Mass Fraction

#### SUBSCRIPTS

- i - Gas Component
- j - Momentum Cell
- k - Mass Cell
- o - Value at  $t=0$