A Hybrid Model of a Gas-Metal Atomizer and its Application to the Development of a Knowledge-Based Control System

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Abstract: A process model has been developed for predicting the dynamic response of a supersonic inert gas-A process model has been developed for predicting the dynamic response of a gas-metal atomizer at the National Institute of Standards and Technology. Both first-principle formulations and empirical correlations of the various atomizer subsystems were incorporated into the model. The process model is capable of predicting the dynamic behavior of process parameters (i.e., temperatures, pressures, gas and liquid flowrates, etc.).

The model is based on a dual control volume formulation (i.e., independent atomizing and melting chambers) for which coupled mass and energy balances have been taken. The various heat and mass fluxes into and out of the control volumes are calculated by means of first-principle relations or empirical correlations obtained from experimental data. From this analysis results a system of coupled equations that is advanced in time using an explicit formulation while responding to a simulated time sequence of process control commands.

The process model allows for the study of possible atomizer modifications and the testing of *what if* scenarios at minimal cost. The paper describes the methodology used in the development of the process model and it suggests how it may be employed for the development of similar models for other types of atomizers.

1. INTRODUCTION

The development of control strategies for a complex industrial process generally requires an iterative process that can be costly, both in time and money. A more economical way to study the dynamic behavior of an industrial artifact is to develop a process model of the system under consideration. The process model is typically a hybrid collection of empirical- and/or first principle-formulations that describes the time dependent behavior of selected inputs and outputs in the system. Once the process model is implemented in a computational environment and validated using actual data, the model can be used to test a large number of control strategies within a reasonable time frame and at a minimal cost.

Gas metal atomization is an industrial process well suited for process modeling. The high operational cost of atomizers and the harsh conditions present in them makes all but impossible the study of their dynamic behavior *in situ*. This paper reviews the procedure used in the development of a process model for the supersonic inert gas-metal atomizer (SiGMA) at the National Institute of Standards and Technology (NIST). The methodology here described, should apply to most atomizers with minor modifications to reflect changes in any particular site.

2. PROCESS MODELING of SiGMA

The first step in the development of the process model for the NIST atomizer was to determine the important process parameters by system identification. The process of *system identification* involves the determination of the process parameters that affect the quality of the process output. Given that system identification involves steps that are not clearly defined, the process is usually an iterative one.

Figure 1 shows the system identification diagram for the SiGMA atomizer. This diagram contains a collection of all the sensors and actuators present in the atomizer today, as well as some process parameters that have been identified to have some effect on the production of powder (e.g., mass flow rates).[1]

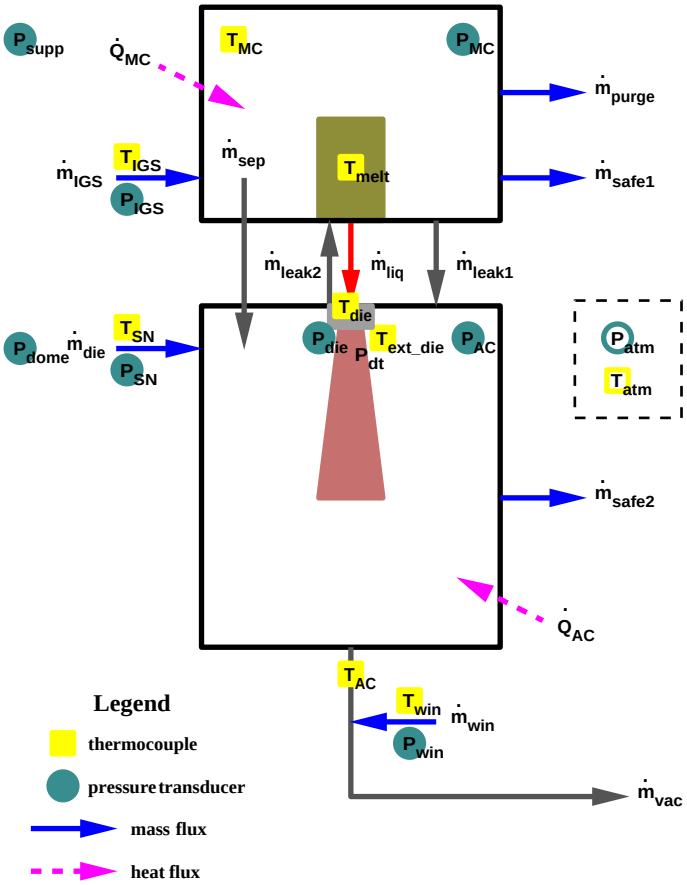

Figure 1. System Identification Diagram of SiGMA.

In the atomizer melting chamber (the upper chamber in Figure 1), thermocouples are used to measure the temperatures of the liquid metal and of the inert gas, while a pressure transducer is used to measure the pressure of the inert gas. In addition, an assortment of thermocouples and pressure transducers is used in conjunction with calibrated sonic nozzles to measure the mass fluxes of gas, into and out of the chamber. This collection of sensors allows for the determination of the thermodynamic state of both the gas ($P_{MC},\ T_{MC}$), and the liquid metal ($P_{MC},\ T_{melt}$), and their rates of change with respect to time (i.e., $\partial P_{MC}/\partial t$, $\partial T_{MC}/\partial t$, and $\partial T_{melt}/\partial t$).

In the atomizing chamber (the lower chamber), sensors to measure pressure and temperature are used to determine the thermodynamic state of the inert gas while the mass fluxes of gas into the chamber are monitored by several sonic nozzle meters. Ideally this, will lead to the determination of the time rates of change of the mass and the energy in the chamber. However, the lack of means to measure the mass flow rate of the liquid, and the mass of gas displaced by the vacuum cleaners, makes the computation of the time derivatives of the state variables impossible. A sensor to measure either of these quantities is needed to improve the monitoring of this chamber.

The remaining parameters in Figure 1 are either process sensors not attached to one of the chambers (e.g., the supply gas manifold pressure, P_{supp}), or parameters that can be derived from the measurements of other sensors (e.g., the aspiration pressure, P_{dt} [1]).

2.1 Mathematical Modeling of SiGMA

The two mayor requirements that a process model must satisfy are: 1) it should describe the dynamic behavior of the system, and 2) it should interact with the process controller in a way that mimics the real system (i.e., it should exhibit the same time lags as the sensors and actuators in the system). Once such a controller is available, the control system can be connected to it and trained over a large number of training periods. The resulting controller will be able to react to events in the real system as well as the process model approximates the real system. Final adjustments to the controller will result from its interaction with the real system during processing.

Seeking such a process model, a dual control volume, mathematical simulator of SiGMA was created. For this model the melt chamber and the atomization chamber were treated as separate control volumes for which mass and energy balances were written. Mass fluxes into and out of the control volumes were accounted for by means of first principle relations. Quantities for which first principle relationships were not available, were modeled using correlations of empirical data (e.g., the aspiration pressure model [1]). Finally, the two control volumes were coupled by means of mass and energy transfers between them.

The control volume formulations yielded a set of four partial differential equations for the rate of change of two independent thermodynamic properties (i.e., temperature and density) in each of the control volumes. The following are examples of the differential equations used to describe the melt chamber control volume. Two similar equations described the behavior of the atomizing chamber (i.e., $\partial \rho_{AC}/\partial t$ and $\partial T_{AC}/\partial t$).

$$\frac{\partial \rho_{MC}}{\partial t} = \frac{1}{V_{MC}} \Big[\dot{m}_{IGS} + \dot{m}_{leak_2} - \dot{m}_{sep} - \dot{m}_{liq} - \dot{m}_{purge} - \dot{m}_{leak_1} - \dot{m}_{safe_1} - \rho_{liq} \frac{\partial V_{liq}}{\partial t} - \rho_{MC} \frac{\partial V_{MC}}{\partial t} \Big] \tag{1}$$

$$\begin{aligned} \frac{\partial T_{MC}}{\partial t} = & \frac{1}{\rho_{MC} c_v V_{MC}} \Bigg\{ \left[c_p T_{IGS} \right] \dot{m}_{IGS} + \left[c_p T_e \right] \dot{m}_{leak_2} \\ & - \left[c_p \frac{T_{MC} + T_{AC}}{2} + \left(\frac{P_{MC}}{\rho_{MC}} - \frac{P_{AC}}{\rho_{AC}} \right) \right] \dot{m}_{sep} - \left[c_l T_l + \frac{P_{MC} - P_{dt}}{\rho_l} \right] \dot{m}_l \\ & - \left[c_p T_{purge} \right] \dot{m}_{purge} - \left[c_p \frac{T_{MC} + T_{AC}}{2} + \left(\frac{P_{MC}}{\rho_{MC}} - \frac{P_{AC}}{\rho_{AC}} \right) \right] \dot{m}_{leak_1} \\ & - \left[c_p T_{MC} + \frac{P_{MC} - P_{atm}}{\rho_{MC}} \right] \dot{m}_{safe_1} - V_{MC} c_v T_{MC} \frac{\partial \rho_{MC}}{\partial t} \\ & - \rho_{MC} c_v T_{MC} \frac{\partial V_{MC}}{\partial t} - \rho_l c_l T_l \frac{\partial V_l}{\partial t} + \dot{Q}_{MC} \Bigg\} \end{aligned} \tag{2}$$

These equations, and their equivalents for the atomization chamber, were discretized in time, using first order finite difference approximations, and the resulting set of ordinary differential equations was advanced in time using Taylor series expansions.

$$\rho_{MC}^{n+1} = \rho_{MC}^{n} + \left(\frac{\partial \rho_{MC}}{\partial t} \right)_n \Delta t + O(\Delta t^2) \tag{3}$$

$$T_{MC}^{n+1} = T_{MC}^{n} + \left(\frac{\partial T_{MC}}{\partial t} \right)_n \Delta t + O(\Delta t^2) \tag{4}$$

$$\rho_{AC}^{n+1} = \rho_{AC}^{n} + \left(\frac{\partial \rho_{AC}}{\partial t} \right)_n \Delta t + O(\Delta t^2) \tag{5}$$

$$T_{AC}^{n+1} = T_{AC}^{n} + \left(\frac{\partial T_{AC}}{\partial t} \right)_n \Delta t + O(\Delta t^2) \tag{6}$$

3. RESULTS & DISCUSSION

The simulator was tested against data obtained from the atomizer during various runs. Each sub-model in the simulator contained a *correction factor* which allowed an adjustment in its performance. During testing, the state variables in the simulator were initialized with the initial data for an atomization run and then the prediction of the model was compared with the performance of the atomizer for that run. The various correction factors were adjusted to obtain the best possible performance over the entire atomization run and the calibration process was repeated with several different atomization runs. The various values for each correction factor, which resulted from all the calibration experiments, were averaged to obtain an overall constant for the NIST atomizer.

The simulator predictions for the temperature and density in the melt chamber control volume were within ±5%, over the entire time of an atomization run (usually about 2.5 min.). For the atomizing chamber the prediction was not satisfactory (±20%) due to the poor estimates in the performance of the vacuum cleaners that extract the waste gas from the NIST atomizer (see Figure 1). This adverse result prompted the installation of a mass flow rate sensor, at the exit of the atomization chamber, to obtain a better model for the vacuum cleaners. This problem in the atomizing chamber prediction would not affect blowout atomizers (i.e., without vacuum cleaners), given that the modeling of these units can be predicted using first principles. With the new flow meter for the gas flow in place, performance comparable to those obtained in the upper chamber is expected from the atomizing chamber in the simulator.

References:

[1] Ridder S.D., Osella S.A., Espina P.I., and Biancaniello F.S., *Inter. J. of Powder Metall.* **28** (1992) 133-147.