Dynamic Analysis of Process Reactors

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ABSTRACT

The process design for integration of advanced gasifiers for combined-cycle facilities requires a dynamic analysis tool for predicting the gasifier performance and stability. Such a tool provides an understanding of both process reactions and the interaction of process components. To illustrate the utility of the process dynamic tool, a Gasifier Dynamic Model (GDM) was developed at the Morgantown Energy Technology Center (METC) to investigate alternative designs and operational scenarios during process design development.

Empirical data and first principles were combined into steady-state process models to develop sensitivity parameters around a nominal process design condition. These gain factors were then coupled with time-dependent functions for process mass and energy inventories to develop the dynamic model (GDM). Engineering calculations performed in the GDM were used to predict process responses such as gas make, flow, pressure, and temperature.

Small research facilities were constructed and operated to validate both the steady-state process and dynamic models. GDM predictions provided engineers insights into the design integrity and operational safety of the reactions, components, and control elements.

INTRODUCTION

METC is involved in the design of an advanced, hybrid coal gasifier based on the PyGas^{TM} process (Carson et al., 1994). This process incorporates a centrally located, jetting, fluid-bed pyrolyzer to mitigate the caking of bituminous coals and a concentric, counterflow, moving-bed section to gasify the remaining carbon (Figure 1). The complexities involved in integrating these reaction components into a single vessel demand an advanced analysis method for process design, operation, and control. This method combined steady-state parameter estimation and process dynamic modeling. The resulting model was a gasifier process simulator for control strategy evaluation.

In the first step of the control analysis, steady-state process models were used to calculate lumped parameter, input-output gain factors. Sensitivity analysis on these models yielded qualitative insights into the dominant reactions as well as mass and energy transfer mechanisms at nominal gasifier operating conditions. The steady-state process models work by converging solutions of the non-linear, mechanistic equations for reactions and dynamics of the jetting fluidized-bed pyrolyzer and the moving-bed gasifier sections of the PyGas^{TM} concept. The localized gain coefficients, attained from exercising the process models, were the key inputs as gain parameters to the GDM.

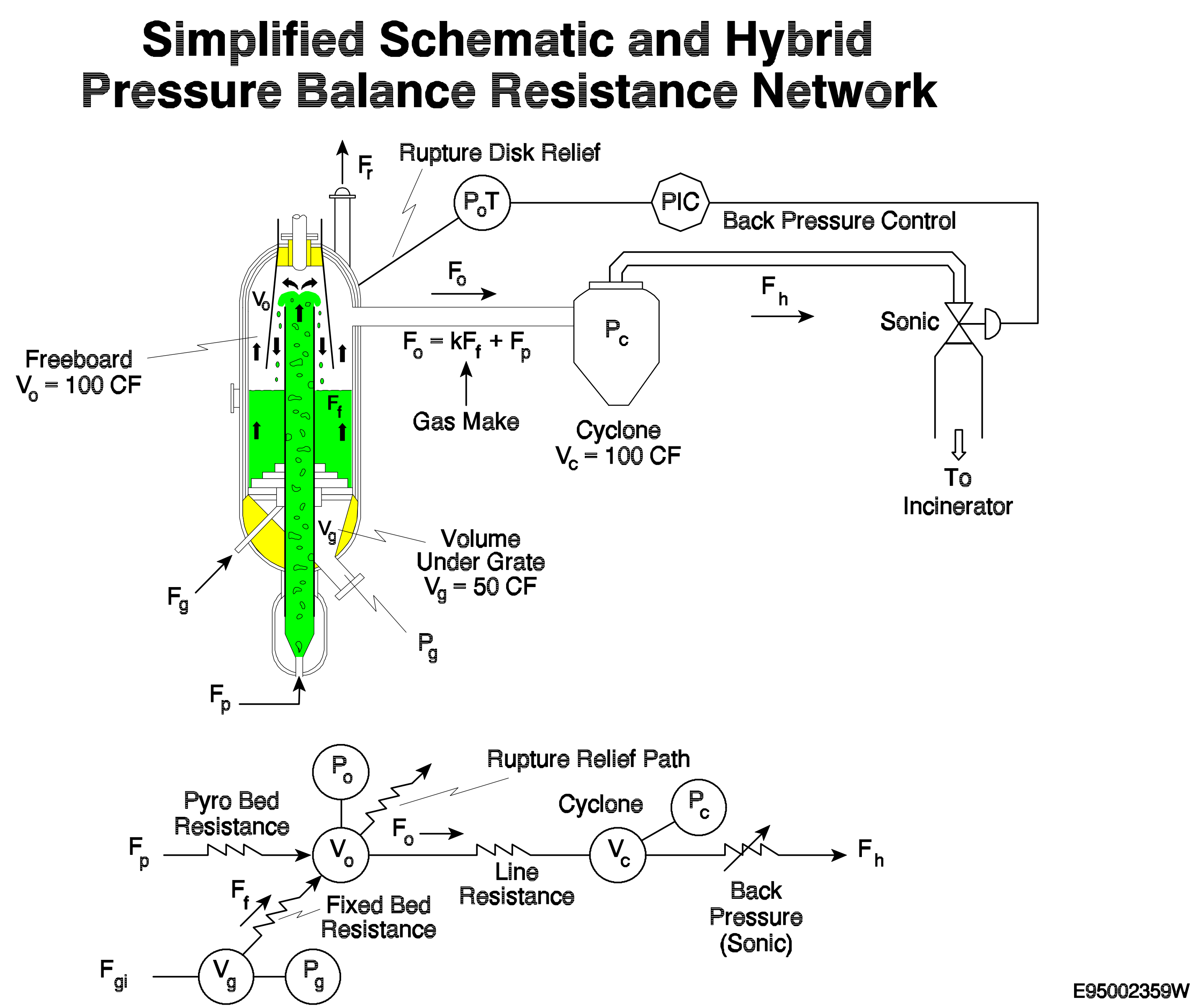

Figure 1. Simplified Schematic and Hybrid Pressure Balance Resistance Network

The integrated dynamic model was developed from the global process phenomena of the integrated design. The equations for the chemical, physical, or thermodynamic mechanisms were defined for interactions between the process variables. The previously identified gain factors were combined with the heat and material inventory capacitances to define a differential equation. Solution of this system of equations would be difficult in closed form, but a computational simulation of each term of the equations enabled the analysis. The GDM, thus simulating process dynamics, was coupled with control strategies to test operational scenarios.

To gain confidence in the predictive capability of both the steady-state and the dynamic models, validation data are being obtained from reactor facility tests at METC. These research facilities include: (1) a one-half scale, plastic, cold-flow model of the PyGas™ gasifier; (2) a 10-inch jetting, fluid-bed coal gasifier; and (3) a pressurized, fixed-bed, char gasification pot which is currently under design.

There is timely utility in performing the dynamic analysis of operational scenarios, instrument placement, and process design prior to construction and operation. The results of simulation yield a measure of control effectiveness. The objective of the dynamic analyses was to test transients in measured or controlled parameters against design constraints and thresholds during operational disturbances. These disturbances may include internal reaction upsets, changes in load variables, and changes in inlet conditions. The dynamic engineering model has also been adapted to the form of a process simulator for off-line training of operators to recognize process disturbances.

PREDICTIVE PROCESS MODELS

Consider first the process models which predict the steady-state performance of the gasifier and from which gain coefficients were derived for the dynamic model. The pyrolyzer model was developed by METC specifically for this application because no commercial software met all the requirements (e.g. hydrodynamics and chemical kinetics) needed for this process. Modeling requirements included reactions that do not achieve equilibrium, spatial voidage, jet height, carbon conversion, thermal equilibrium, pressure profile, and superficial velocities.

The model of the complete, integrated process is called the PyGas™ Heuristic Automatic Modeling Executive model or PHAME (Trapp 1994). PHAME executes three models that represent the three zones in the gasifier where streams are introduced. The three zones are the pyrolyzer, the top and co-flow, and the fixed bed. Although they are separate, these zones depend upon and interact with each other. As would be anticipated, these models do not converge to state-space balance in real-time nor do they compute time-dependent functions.

The first model, JET, was used to simulate the jetting, fluid-bed pyrolyzer (Noel et al., 1995). A mass and energy balance was calculated for the given coal composition considering, volatile matter and tar compositions. All major gasification and combustion reactions that apply were considered; however, only the water-gas shift reaction was allowed to reach equilibrium. To better represent a gasifier, some empirical functions were introduced into the model. Empirical functions were developed based on Foster Wheeler carbonizer test data to determine the amount of volatile matter that reacts with inlet air and the amount of char gasification in the jet (Archer and LaNeve, 1994).

The JET model also includes empirical hydrodynamic parameters. These parameters include jet penetration (Yang and Keairns 1982), char recirculation into the jet, superficial velocities of solids and gases, and fluidization regime (Yang et al., 1986). The model's results were favorably matched with Foster Wheeler carbonizer (Katta, et al. 1988), KRW gasifier (Froehlich et al., 1994), and METC fluid-bed gasifier data (Rockey et al., 1995). Conversion, gas heating value, and process temperatures were readily matched based on experimental, nominal operating inlet flows by adjusting several indirect parameters, but agreement between model and experimental gas compositions as constrained by the water-gas shift equilibrium was only fair. Since the operating conditions for the pyrolyzer most closely approximate those of the Foster Wheeler carbonizer, it was decided to fix the adjustable indirect parameters based on the best match with that data.

The outputs from the pyrolyzer model and any air introduced into the top combustor were used as inputs into the top and co-flow model in PHAME. This model was developed using the METC Gasifier Advanced Simulation (MGAS) (Syamlal and Bissett 1992). MGAS describes a gasifier in terms of a gas phase and a solids (coal or char) phase and considers coal combustion, steam and CO_2 gasification, methanation, water-gas shift, volatile evolution, tar cracking, and gas phase combustion reactions. The kinetic rate expressions for the gasification reactions were taken from Wen et al.(1982). In MGAS, a set of mass balance equations and energy balance equations are solved for the gas and the solids phases. The solution of these equations gives the time-dependent, one-dimensional distribution of species mass fractions, and temperatures.

Simulations of METC, Wellman-Galusha, General Electric, and Lurgi/Westfield gasifiers (Thimsen and Maurer, 1990) were done using MGAS for code validation purposes. The steady-state values of the product gas flow rates, composition, and temperature calculated by MGAS were found to be in reasonable agreement with the experimental data.

The outputs from the top and co-flow zones of the gasifier, and any air or steam introduced into the grate were input to a second MGAS model set up to simulate the countercurrent fixed-bed configuration. This second MGAS model was configured to accurately simulate the geometric entrance of streams into the gasifier. The solid material coming out of the co-flow zones was the only stream considered to enter into the top of the fixed-bed model. The gases exiting from the co-flow zone were mixed with the exit gases from the counterflow fixed-bed by PHAME to best represent the total gasifier outlet gas.

STEADY-STATE PROCESS GAIN FACTORS

Process control development first requires characterization of the process sensitivities to inputs. Since this gasifier design is an experimental process, prediction of gasifier behavior is speculative. Computer simulations gave computational insight into the reactor's performance and behavior. Multiple sensitivity studies were conducted using output from steady-state predictive models to provide key transfer-function gains (input/output). Obviously, the extensive, spatially distributed calculations in the models described above do not execute to converge in real time. Thus, a macro-process model was formulated from the sensitivity analysis of these models to achieve a real-time simulation. The transfer functions resulting from the parametric sensitivities served to reduce the spatially dependent factors to lumped parameters in the macro. See Figure 1 of illustrated components and an analogous network representation of lumped parameters.

The approach taken was to assume that the complex process functions can be linearized as lumped parameters once the relative effects were quantified through parametric sensitivities. Sensitivities were performed over a narrow range around the expected operating point in order to choose several possible control schemes. Where nonlinear functions were known over a wider operating range, they were included in the dynamic model and tested in the steady state for validation. Only by the use of a dynamic model, can a final control scheme be chosen.

For this analysis, only measurable output parameters such as temperatures, gas flow, and gas compositions were considered around a nominal operating condition. All flows were taken from nominal design heat and material balance calculations. Gas-make was calculated as a lumped parameter from the ratio of output to input stoichiometric mass flow balances. The benefit to experimenters and operators of models' integration is in understanding the scale of these process parameters.

Localized linearization was done by using the steady-state predictive model results observed from runs with a 5 percent change of each manipulated variable around (localized to) the operating point. The gains were calculated by the ratio of measured variable change to the manipulated variable change.

TIME-DEPENDENT DYNAMIC TERMS

The steady-state process model does not represent time-dependent functions inherent in the process and so cannot simulate transient characteristics. The dominant time-dependent functions were derived from the dynamic driving and convergence mechanisms in the GDM. Capacitance for heat and material in the process are time rate parameters that determine inventory as a function of time. Capacitances were determined for the process reactor geometric dimensions and material properties (specific heat and density). The equations which balance time-dependent inventory building with inventory removal were expressed in terms of the time functions. The parameters of inventory gain or loss due to the process variables (pressure, flow, gas make, and temperature) were taken as those determined from the steady-state process models.

Each coefficient in a set of differential equations represents a process parameter. These systems of equations, once solved in closed form, would yield a characteristic process state. But this mathematical complexity makes an alternative, simulation method more attractive. Simulation in the time domain reveals more of the response than would a single process state. The time domain simulation engages the process engineer. The system of equations that describes gasifier dynamics simulates transient responses to changes in input conditions (flows and pressures) as well as changes in internal process parameters (bed resistance and control valve position) as these parameters change through time.

MEANS OF SIMULATION

The representational structure of the commercial TUTSIM model used in this study allowed additional mathematical expressions to be added as modules of computational blocks shown in Figure 2. In each block the individual terms in the system of equations described above were computed. As the computation proceeds, the time-dependent functions in the model drive the system of interconnected computational blocks to simulate difference equations of mass and energy balance equations. Each connecting line represents a time-dependent process variable. Chains of model function blocks and connecting lines form loops which couple processes on themselves.

REAL-TIME SIMULATION

If the speed of the computer is sufficient to execute simulation time steps on an actual time scale, the model then becomes capable of real-time simulation of the process. Obviously, if rapid dynamics are inherent, a slower than real-time simulation has the advantage of expanding time for observation. Conversely, if slow dynamics are prevalent, compression of time helps to observe long time responses. If an objective is to test interaction between the simulated process, control systems and operators, a real-time simulation is needed. Simulations of the gasifier have shown utility for all three treatments of time.

PRESSURE PROFILE DYNAMICS

A gas pressure profile dynamic originates from a dependence between the stored volume of gas in the gasifier, the rate of gas production, and the pressure dependence of the exiting flow rate function. Capacitance terms in the dynamic model provide the time-dependent functions needed to simulate the pressure balance coupling between cyclone volume, back pressure valve, fixed-bed gas production, and pyrolyzer gas production (Figure 1).

The model was centered around the common freeboard volume of the gasifier. The product gas from the fluidized-bed pyrolyzer and the fixed bed contribute gas flow in response to input air flows. It was assumed that each bed acts as a readily available supply of solid fuel, and that changes from the nominal inlet air flows have an immediate, proportional deviation on the gas production rates. This assumption is valid due to the small time constant of gas production relative to pressure deviations of gas inventory in the freeboard.

The air flow to the fixed bed was found to be a function of the pressure drop across the flow resistance of the fixed bed. The driving pressure is a time-dependent function of the inventory of gas above the bed, in the freeboard, and below the grate. Further, an under grate volume present between the inlet streams and the fixed bed resulted in a time lag between manipulation of input air flow and actual air flow within the fixed bed.

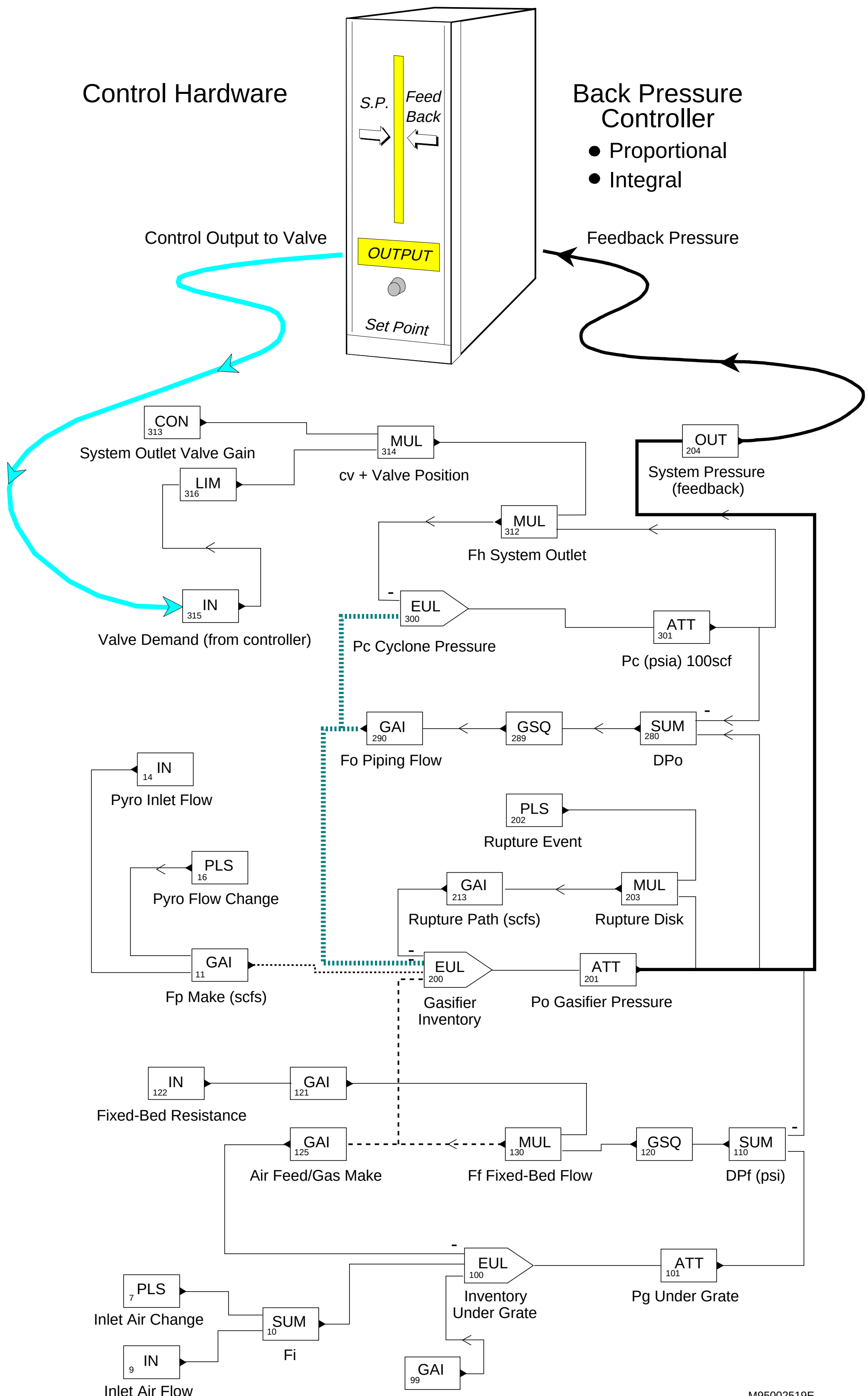

Figure 2. Dynamic Model Simulator

Likewise for the fluidized bed, a resistance function of pressure drop with flow through the bed was incorporated but assumes no inventory volume under the bed. It is important to understand that the increase in flow through a fluid bed results in **decreased** pressure drop across the bed due to increased void fraction. This effectively represented a negative dynamic bed resistance. Complex, mixed-phase dynamics were expected to take place as spatially distributed functions within the fluid bed, but the resulting pressure and flow functions were generally considered rapid compared to gasifier inventory derived terms. The fluid-bed resistance was reduced to a single, lumped parameter in the Gasifier Dynamic Simulation.

RESULTING PRESSURE AND FLOW RESPONSES

The under grate pressure, Pg of Figure 3, responded smoothly to an imposed 2 scfs increase of the air flow under the grate, Fi. The freeboard outlet flow, Fo, similarly responded with a rise to the eventual, new flow balance seen in Figure 4. This appeared to be a first-order response, but was, in fact, a coupled response of the under grate inventory and freeboard inventory.

The effect of imposing 2 scfs increase in pyrolyzer inlet air flow, Fp, resulted in an abrupt freeboard outlet flow, Fo, of Figure 5. The magnitude of deviation in the freeboard outlet flow, Fo, in Figure 5 was similar to the response to the previous change in the fixed-bed, Fg. The response, however, was more immediate due to the small relative volume and gas residence time in the pyrolyzer. In response to the same increased pyrolyzer flow, a negative going, transient decrease in fixed-bed flow, Fg, was observed (Figure 6). This inverse response of fixed-bed flow was due to an increase in system back pressure due, in turn, leading to increased total outlet flow across the outlet resistance. It is interesting to note that the eventual recovery of original fixed-bed flow, Fg, corresponded to the eventual new pressure and flow balances.

It would be difficult to calculate the effect chages in flow rates on the time-dependent balance in system pressure. But the dynamic model allowed simulation to attain the computational balance and frees the observer to understand the resulting effects.

THERMAL MODEL DYNAMICS

With a gas inventory model established, the next dominant mechanism anticipated was the evolution and removal of heat from the fixed bed. The thermodynamic control volume to be modeled was that of the entire bed mass as a constant. The inventory of solids was assumed to be readily available for reaction with air to produce heat. Thus, the incremental amount of heat produced was proportional to the deviation in air flow from the nominal. The thermal model became an additional module of difference equations that utilize the existing flow balancing structure. The resulting temperature variable became a compensating term to the gas density computation. In this way the model quickly begins to capture and represent the coupled dynamics of both gas and thermal inventories. The relative time constant of the thermal model was found to be long (hundreds of seconds) compared to the volumetric time constant of the gas inventory (tens of seconds).

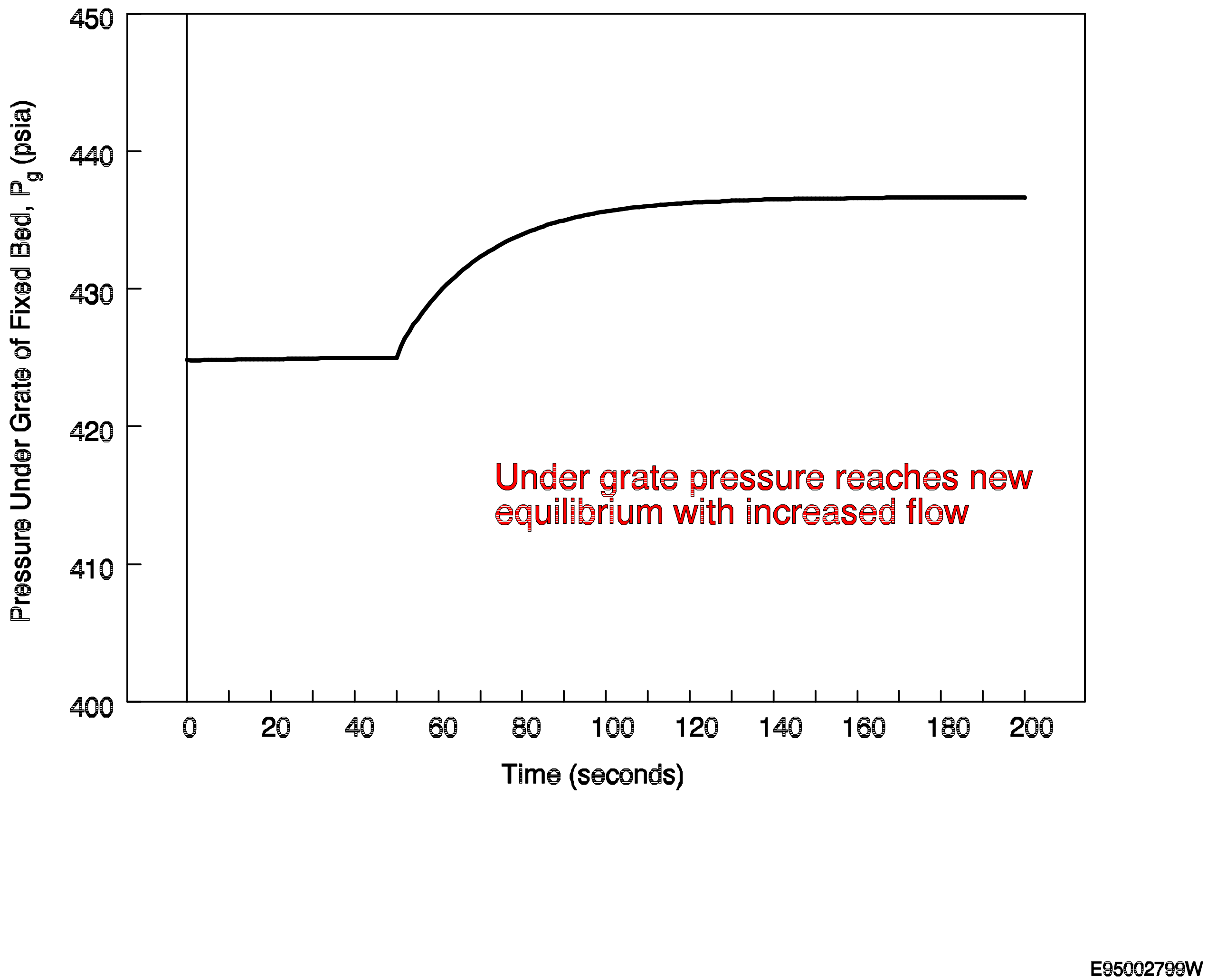

Figure 3. P_g Response to Step Increase of F_i at Time $t = 50$ sec

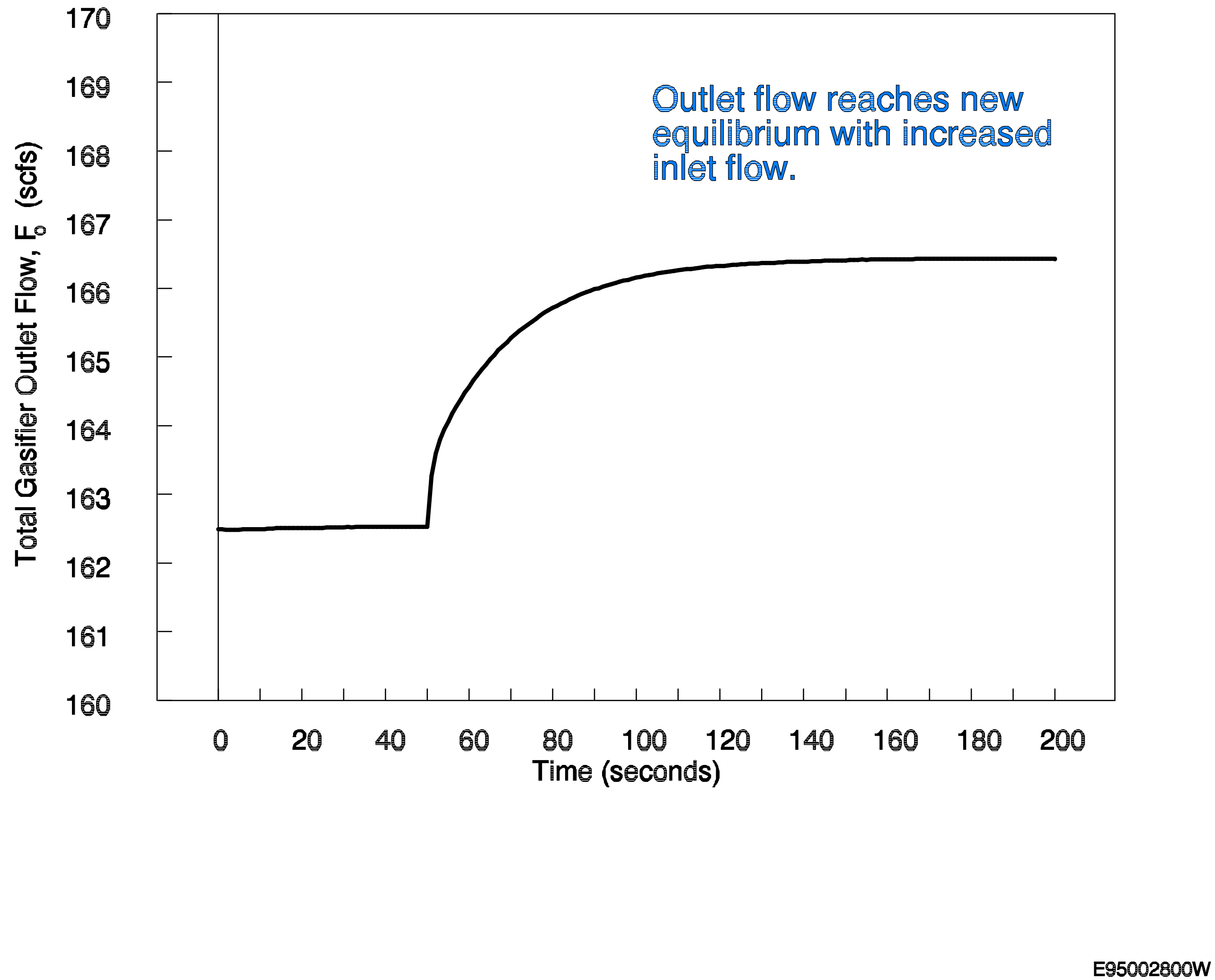

Figure 4. F_o Response to Step Increase of F_i at Time $t = 50$ sec

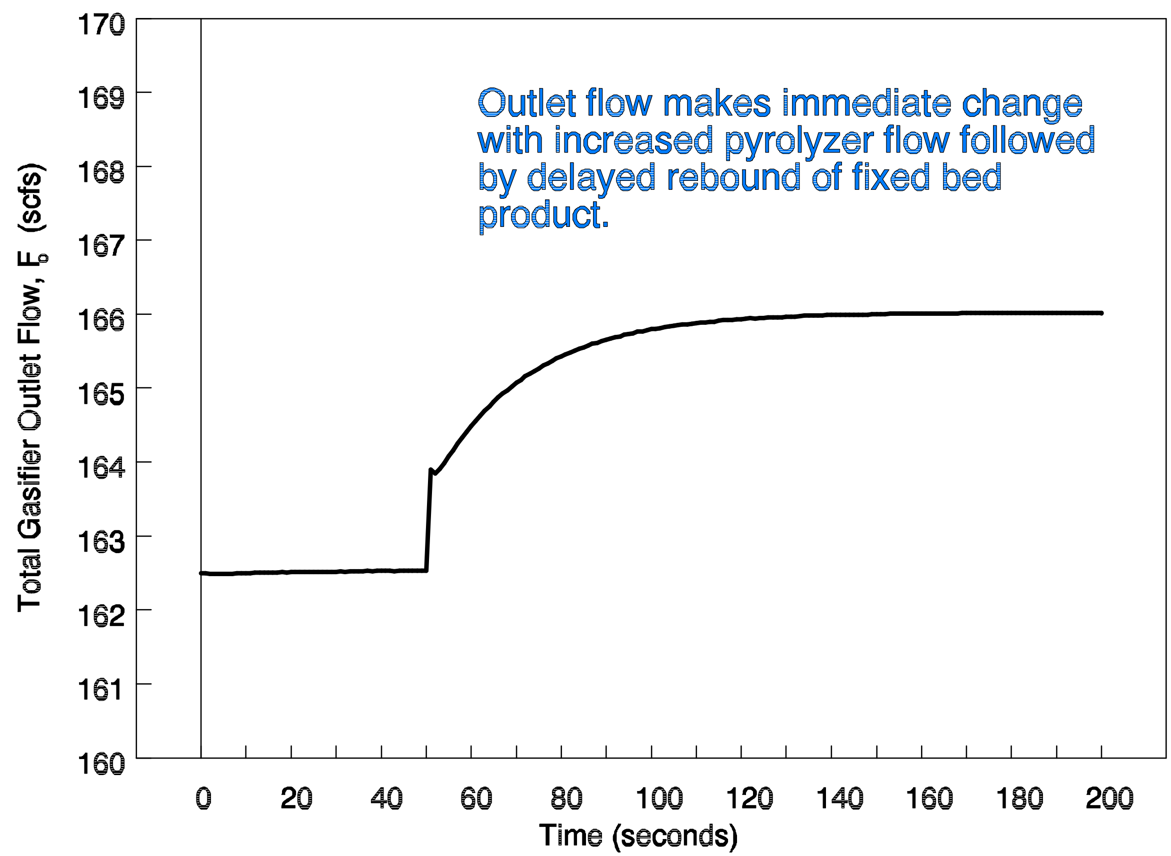

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Figure 5. F_o Response to Step Increase of F_p at Time $t = 50$ sec

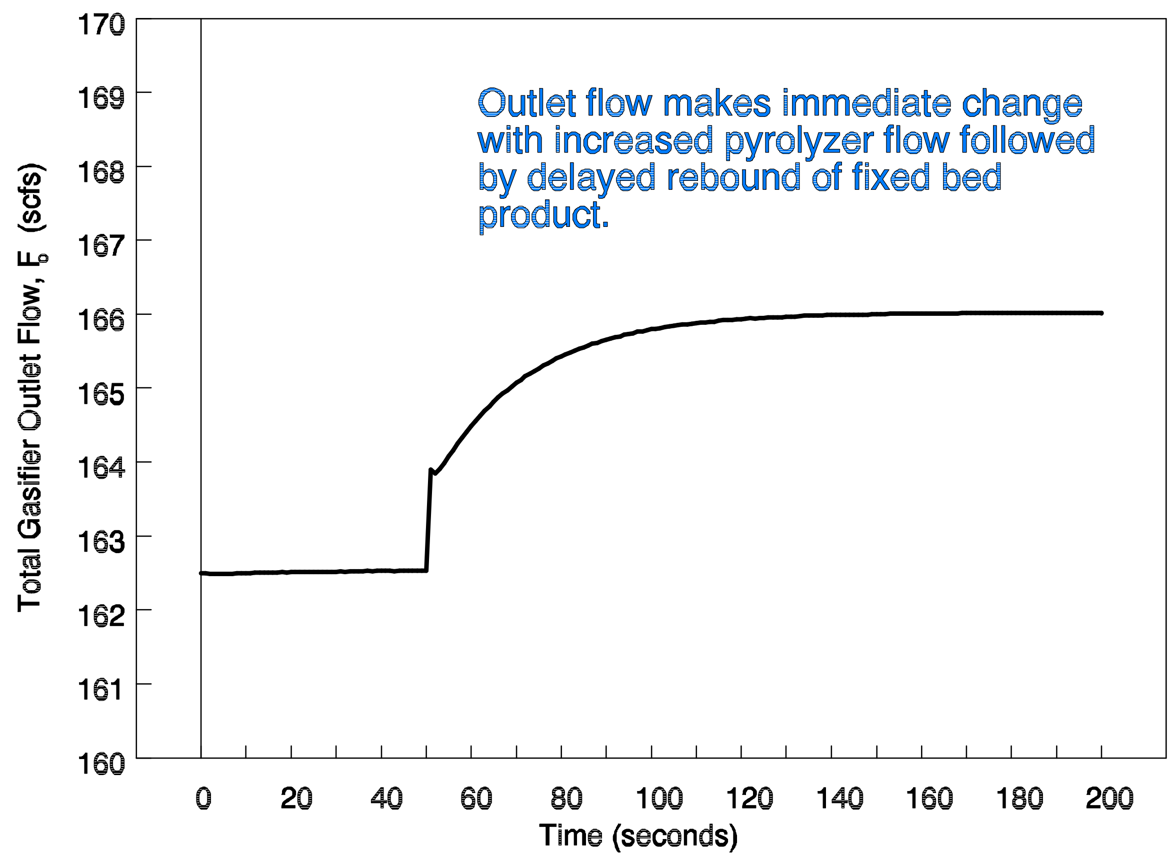

Figure 6. F_g Response to Step Increase of F_p at Time t = 50 sec

STEAM DRUM DYNAMIC MODEL

An important dynamic aspect of a water-cooled gasifier was the interaction of the gasifier pressure with the cooling water jacket circuits and steam drum pressure. An adaptive extension of the dynamic model tested the stability of the mechanisms of steam production in the steam drum as they couple to pressure transients in the gasifier. A self-passivization shutdown scenario would rely on stable pressure balance between the gasifier pressure and water jacket steam drum.

Time-dependent terms arose from the inventory of water, steam, and heat energy in the jacket and drum as a function of steam conditions. Steam conditions were, in turn, a function of temperature and pressure. The drum system was represented as a system of coupled mass and energy balance equations and simulated by a additional dynamic module to the GDM.

Two mechanisms couple the gasifier with the water jacket system. First, heat transfer through the wall to the water jacket coupled to steam generation in the steam drum. Second, the steam generated in the jacket drum flowed (through a suitably sized fixed orifice) to the pyrolyzer and grate zones of the gasifier for inerting the reactions and sustaining a small pressure differential between the water jacket and the gasifier during shutdown depressurization cases.

The modular structure of the GDM allowed the addition of suitable steam drum dynamics to identify the worst case scenario by testing for violation of thermal shock and mechanical stress constraints.

FUTURE INTEGRATION OF MODULES

Variations of the dynamic model currently under development at METC were needed to validate single-loop and multi-loop control schemes. As a result, the product gas temperature emerging from the pyrolyzer and fixed-bed regions, presently constant parameters, can be modeled as coupled variables between the thermal model and the pressure profile model. As a tool for process design, the objective was to test design parameters that were not yet cast in concrete and steel.

There is a great likelihood that as positive coupling mechanisms are added, second-order dynamics will result in instabilities. Care must be taken to rank the relative coupling gains of various modules so as to recognize when one mechanism dominates or "swamps" the effects of others.

The resulting dynamic process simulation of transients can show breeches in mechanical or physical constraints, system instabilities leading to divergence from steady-state, undesired side effects, and excessively long thermal time constants relative to shorter, desired balancing mechanisms. The process of testing and discovery allows thorough design and testing of the process control scheme before the process parameters (due to geometric dimensions) are cast into a fabrication design.

The model helps one to understand which process variables are important but not directly measurable, thus helping to define process instrumentation needs. The exercises of the model help to define the operational test matrix to validate process performance. For process variables that are not directly measurable, on-line dynamic computations can infer process data that is not directly observable.

EXPERIMENTAL VALIDATION

A one-half scale, plastic, cold flow model was fabricated and is being operated to demonstrate the fluid dynamics of the PyGas™ concept. This model includes components including the pyrolyzer tube, a rotating grate used to support and distribute air through a counterflow fixed bed, and a freeboard annular gas exit region. The cold flow unit has a 30-inch inner diameter, a 10-foot external shell, and a hemispherical dome on top. The model is capable of being operated with continuous solids and gas flow at conditions scaled from the process design. This unit is being operated to provide data to validate the process model estimates of fluid dynamic behavior in the hot unit.

A second research facility being used to validate the models is the METC 10-inch fluid-bed gasifier system which consists of a pressurized (425 psig) gasifier and several subsystems, e.g., coal storage conveying system, air preheater, particulate removal system, and an incinerator. The gasifier is a 20-foot high, nominal 80 lb/hr, air-blown and refractory-lined vessel. Coal is fed into the gasifier by ambient (convey) air through the center core of a concentric nozzle located at the bottom of the bed. Preheated (reactor) air and steam are premixed and introduced into the bed through the annular core of the nozzle. This system produces about 300 lb/hr of flue gas with a heating value of 120 Btu/scf. This gasifier has provided operational data to verify predictive process models, and it is being used to test and verify advanced control schemes.

A third research reactor for model validation is the Pressurized Gasification Pot (PGP). The PGP will be 2 feet in diameter and 5 feet in height, with an inner diameter of 1 foot for the fixed-bed reactor and refractory surrounding it. The unit will be operated up to 600 psi, 1,600 °F, gasifying coke and char generated from the above described, fluidized-bed gasifier. The offgas of the gasification pot will flow to a gas chromatograph for gas analysis. Data collected on char conversion rate, gas production, and other performance factors will be used to validate the fixed-bed process models.

CONCLUSIONS

The models described have a primary benefit of providing the process control engineer the means of understanding the critical process interactions. They have already enabled testing of alternative control strategies for the PyGas™ gasifier. Although modeling codes were initially developed to optimize a control scheme, they will have utility throughout the operational life of the process for model based process control.

Longer term modeling applications involve optimization of the gasification process. Operations will be simplified by uncoupling the hybrid reactor components' responses to inlet changes through control scheme development. Operational surprises will be minimized by anticipating the process response to inlet changes.

The model has become a suitable simulator for testing and tuning the control loops prior to plant start-up. As an off-line simulator, the model may act as a training simulator for operators. As an on-line simulator, once validated, the model may prove useful as an operational tool in diagnosing operational problems such as bed channeling, clinker agglomeration, and bed slugging.

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