A TWO-PARAMETER PRELIMINARY OPTIMIZATION STUDY FOR A FLUIDIZED-BED BOILER THROUGH A COMPREHENSIVE MATHEMATICAL SIMULATOR

José A. Rabi – jrabi@fem.unicamp.br Márcio L. de Souza-Santos – dss@fem.unicamp.br UNICAMP – State University at Campinas, Faculty of Mechanical Engineering, Department of Energy, Cx. P. 6122 – 13083-970 – Campinas, SP, Brazil

Abstract. Modeling and simulation of fluidized-bed equipment have demonstrated their importance as a tool for design and optimization of industrial equipment. Accordingly, this work carries on an optimization study of a fluidized-bed boiler with the aid of a comprehensive mathematical simulator. The configuration data of the boiler are based on a particular Babcock & Wilcox Co. (USA) test unit. Due to their importance, the number of tubes in the bed section and the air excess are chosen as the parameters upon which the optimization study is based. On their turn, the fixed-carbon conversion factor and the boiler efficiency are chosen as two distinct optimization objectives. The results from both preliminary searches are compared. The present work is intended to be just a study on possible routes for future optimization of larger boilers. Nonetheless, the present discussion might give some insight on the equipment behavior.

Keywords: Fluidized-bed boiler, Simulation, Modeling, Optimization

1. INTRODUCTION

The fluidized bed technology has been used since the fifties. By virtue of its attractive features, it is nowadays extensively employed in industrial processes involving combustors, gasifiers and chemical reactors. Among the advantages over more conventional processes, bubbling fluidized-bed equipment allows high degree control of the temperature inside the bed, relatively high heat-transfer coefficients between bed material and immersed tubes, high turn-down rates and low pollutant (NO_x, SO_x and tar) emissions (de Souza-Santos, 1987).

Modeling and simulation of fluidized-bed equipment plays a major role in design and optimization, mainly because experimentation is much more expensive than computation. Besides, numerical procedures may be the only permissible way to explore limiting situations due to safety concerns. Accordingly, a comprehensive mathematical model and computer program should cover important aspects and phenomena of the process and hence they should be able to predict parameters that describe the operation of the equipment.

In this work, a preliminary optimization study of a fluidized-bed boiler is accomplished with the aid of a comprehensive mathematical simulator. The configuration data of the boiler are based on a particular Babcock & Wilcox Co. (1976) test unit. The simulation program has already been tested against experimental data from real operation and the corresponding numerical results generated for several parameters have shown only small deviations (de Souza-Santos, 1987, 1989).

Since there are numerous variables upon which the optimization study could be based, it was decided to restrict it to only two parameters of major importance, namely: the number of tubes in the bed section and the excess of O_2 over the stoichiometric value. On their turn, the fixed-carbon conversion factor and the boiler efficiency were chosen as two distinct optimization objectives. The results from both studies were compared and correlated. Complementary data, such as bubble diameter at the middle of the bed, the total amount of steam generated and the average temperature at the bed center are also presented.

2. MATHEMATICAL MODEL AND SIMULATION PROGRAM

The program simulates steady-state regime operation of a fluidized-bed combustor boiler test unit, whose schematic diagram is shown in Fig. 1. Coal and limestone are continuously fed into the bed. Species taking part in the emulsion phase are: interstitial gas, carbonaceous solid, inert material and limestone. The bubble phase is free of solid particles and the clouds are incorporated in the emulsion phase. Plug-flow regimes are assumed for the gas in the bubble and for the interstitial gas in the emulsion. This kind of flow is also assumed for the gas flow in the freeboard. A schematic representation of the model is presented by Fig. 2.



Figure 1. Schematic diagram of the fluidized-bed boiler simulated.

Devolatilization processes (reactions and mass transfer through the particle) occur in the vicinity of the feeding point. The size of that region is dictated by a balance between the rate of the devolatilization processes and the circulation rate of carbonaceous particles in the bed.

A similar approach determines the region affected by the drying process. Bubble size is also a function of the bed height z. At the region occupied by the tube bank, its maximum diameter is influenced by the horizontal distance between neighboring tubes.



Figure 2. Basic scheme of the mathematical model.

Among the possible available mechanisms, the heterogeneous reactions between gases and the carbonaceous solid are described by exposed-core (or segregated-ash) model. On the other hand, the unreacted-core (or shrinking-core) model is applied for coal devolatilization and sulfur capture by limestone. Those classical models have been generalized for particles of several possible shapes (de Souza-Santos, 1994a).

The basic characteristics and results that can be provided by the program are:

- Concentration profiles of 20 gaseous components (H₂, H₂O, CO, CO₂, O₂, N₂, CH₄, SO₂, NO, NO₂, N₂O, H₂S, NH₃, C₂H₄, C₂H₆, C₃H₆, C₃H₈, C₆H₆, Tar) throughout the bed (emulsion and bubbles) and the freeboard;
- Flow and temperature profiles of gases in the bed and freeboard;
- Temperature, rate of circulation profiles (or flow) of solid phase components in the bed and freeboard;
- Composition, particle size distribution of each solid species in the bed and at each point of the freeboard;
- At each point of the equipment, all important parameters related to the bed and freeboard dynamics, among them: bubble diameters, upward velocities of each phase (emulsion, bubbles, particles), minimum fluidization parameters, rate of particle turnovers, etc.;
- In cases of recycling of solid collected by the cyclones, all parameters describing such operation, as well as its effects in the process;

- Profiles of individual rates of all homogeneous and heterogeneous reactions (around 30 in each phase: emulsion, bubble, freeboard). This can provide a clear picture for deeper understanding of the processes occurring at each point of the equipment;
- Important engineering parameters to help in design as well as optimization of equipment and operations.

Although many improved versions have been developed (de Souza-Santos, 1992a, 1992b, 1992c, 1993a, 1993b, 1994a, 1994b, 1995, 1996a, 1996b, 1997a, 1997b, 1997c, 1997d, 1997e, 1998, de Souza-Santos et al., 1992), the basic system of differential equations resulting from the mass and energy balances throughout the bed and freeboard sections and the simulation strategy can be found in the original work (de Souza-Santos, 1987, 1989).

As far as boundary conditions are concerned, the only set of conditions completely known refers to the gas stream injected through the distributor (z = 0). It is also possible to state the boundary conditions for the lowest part of the freeboard as being the exiting conditions at the top of the bed. However, the boundary conditions for the temperature of each individual solid species at the base of the bed is calculated by a convergence routine based on the heat fluxes transferred by convection and by conduction at z = 0.

3. DESCRIPTION OF THE REAL OPERATION TEST UNIT SIMULATED

The basic necessary input data for the simulation program comprise:

- Physical and chemical characterization of the fed carbonaceous, limestone and inert solids;
- Characterization of the gaseous agent injected through the distributor; and
- Complete description of the equipment geometry.

Comparisons between real operation data and simulation-generated results have shown only small deviations for several parameters (de Souza-Santos, 1987, 1989).

Some basic data regarding plant operation and the equipment are shown in Table 1. These conditions were those held constant over all simulation runs. It is important to mention that the lowest and highest positions of horizontal tubes of the bank immersed in the bed are kept constant. Therefore, for an increasing number of bed tubes, the free space between them is reduced. The number of tubes was limited to 35 due to the available space in the bed.

For this preliminary optimization study, two operational data were chosen as parameters: the number of tubes in the bed section and the O_2 excess over the stoichiometric value. As a matter of fact, this last parameter is determined by the flow rate of air injected into bed through the distributor and its composition. Since the inlet flow rate of carbonaceous solids is kept constant, this last parameter can also be interpreted as a variable air-fuel ratio.

The number of tubes in the bed bank assumed values from 27 and 35. For the O_2 excess, another five values were taken between 19% and 27%, leading to 25 possible combinations. Considering the inlet flow of coal and its composition (Table 1), the flow rate of O_2 for complete or stoichiometric combustion was 0.1287 kg.s⁻¹. Table 2 summarizes the values related to the inlet flow rate of air, which is the second optimization parameter.

4. SIMULATION RESULTS

The two optimization objectives are defined as

fixed - carbon conversion =
$$1 - \frac{\text{fixed} - \text{C content in exiting carbonaceous particles}}{\text{fixed} - \text{C content in feeding carbonaceous particles}}$$
 (1)

Detail	Value		
Coal proximate analysis (wet basis - % mass)			
Moisture	5.0		
Volatiles	38.0		
Fixed carbon	47.6		
Ash	9.4		
Coal ultimate analysis (dry basis - % mass)			
С	73.2		
Н	5.1		
0	7.9		
Ν	0.9		
S	3.0		
Ash	9.9		
Inlet gas through distributor (wet basis - % mass)			
N_2	75.428		
O_2	22.785		
H ₂ O	1.201		
CH_4	0.432		
C_2H_6	0.154		
Boiler basic geometry			
Equivalent diameter: $D_{\rm D} = D_{\rm F}$ (m)	1.118		
Bed height: z_D (m)	0.700		
Freeboard height: z_F (m)	3.442		
Feeding point height: z_{FEED} (m)	0.305		
Tube bank			
Number of tubes in the freeboard	30		
Length of each tube (m)	0.991		
Bottom bed tube position: z_{TUDB} (m)	0.330		
Top bed tube position: z_{TUDT} (m)	0.700		
External diameter (m)	0.0483		
Internal diameter (m)	0.0409		
Number of orifices in distributor	1500		
Flow of coal (kg.s ^{-1})	0.0585		
Flow of limestone $(kg.s^{-1})$	0.01215		

Table 1. Basic data for the B&W unit and operational conditions for test no. 26.

Table 2. Corresponding values for different inlet O_2 excess.

O_2 excess	19%	21%	23%	25%	27%
O_2 mass flow (kg.s ⁻¹)	0.1532	0.1558	0.1583	0.1609	0.1635
Air mass flow (kg.s ^{-1})	0.6723	0.6836	0.6949	0.7062	0.7175
Air-fuel (AF) ratio	11.49	11.68	11.88	12.07	12.26

Roughly speaking, the fixed-carbon conversion is a measure of how much carbon from the feeding coal is converted into the gas. The boiler efficiency indicates the fraction of the inlet energy (fuel combustion enthalpy times its inlet flow) transferred to tube banks for steam generation and/or water heating. Figures 3 and 4 illustrate the results for those parameters within the described range of imposed values for number of tubes and air excesses.

Before starting the discussion, it is important to mention that this study was based on an experimental pilot unit operating at exploratory conditions. Therefore, the boiler efficiencies as well carbon conversions here attained are low when compared to those encountered in industrial boilers. The present work is just an exercise on possible routes for future optimization of larger boilers. A thorough and detailed optimization study for boiler performance goes far beyond the analysis of air excess and number of tubes influences. Nonetheless, the present discussion might give some insight on the equipment behavior.



Figure 3. Results for the fixed-carbon conversion.



Figure 4. Results for the boiler efficiency.

Figure 5 shows the influence of the studied parameters on the bubble diameter at the middle of the bed (z = 0.350 m). As expected, bubble size increases for larger flow rates of air, which corresponds to larger O₂ excess. The program considers the size increase of bubbles due to coalescence (see Fig. 6, obtained for 33 tubes and 23% excess of O₂). However, as they enter the region of tube bank, the distance between neighboring tubes should limit its size. Thus, as the number of tubes increases, smaller bubbles are found at that position.



Figure 5. Bubble diameter at the middle of the bed.



Figure 6. Typical bubble velocity and diameter profiles throughout the bed.

As far as fixed-carbon conversion is concerned, the highest values are found for fewer tubes in the bed bundle and for larger O_2 excess (Fig. 3). Nevertheless, at several rows of constant values for air (or oxygen) excesses, a minimum has been observed within the investigated range of number of tubes. Despite that fact that no differences larger than 1% were observed for this optimization objective variable, that effect can be readily clarified. The carbon conversion tends to increase for beds at higher temperatures and the average

temperature in the bed tends to increase for lower air excesses as well for fewer tubes in the bed, as shown in Fig. 7. Therefore, the carbon conversion should, as a principle, increase for lower air excesses and fewer tubes in the bed. On the other hand and as commented before, the diameter of bubbles tends to decrease if more tubes are immersed in the bed (Fig. 5). Smaller bubbles lead to more efficient mass transfer of oxygen from them to the emulsion. As the carbonaceous particles are found in the emulsion, the carbon conversion tends to increase for beds with smaller bubbles. As seen, the effect of temperature and concentrations of reactants are, in this case, two opposing effects that explain the minimums observed in Fig. 3.







Figure 8. Rate of steam generation.

At several lines of constant number of tubes, Fig. 3 also shows maximums for the carbon conversion within the range of tested O_2 excesses. This can be understood due to 2 conflicting factors. For a constant carbonaceous solid feeding rate, increases in O_2 excess enriches the O_2 atmosphere that helps to accelerate the combustion reaction rate by chemical kinetics rationale. On the other hand, it also augments the flow rate of air and therefore tends to reduce the bed average temperature (Fig. 7) which in turn decrease the above mentioned reaction rate.

Data related to the boiler efficiency (Fig. 4) show peaks for 21% excess of O_2 and larger number of tubes (33 or 35). It should also be noticed that, for the row of 19% oxygen excess, a maximum was found within the studied range of tube numbers. Obviously, higher temperatures (Fig. 7) are achieved for decreasing number of tubes immersed in the bed. As a principle, greater number of tubes leads to higher amount of heat transferred from the bed to the tubes and the overall efficiency of the boiler tends to increase. However, as the bed temperature decreases for larger amount of tubes, so does the rate heat transfer between each tube and the bed. These two conflicting tendencies lead to the maximums observed at the row of constant 19% O_2 excess (Fig. 4). For other rows this does not happen since the maximum for boiler efficiency is located out of the range covered by number of tubes in the bank.

Figure 8 shows the variation of another operational parameter, namely the steam generation rate. The tendency presented in the is readily recognized to follow the one shown for the boiler efficiency plot (Fig. 4).

4. CONCLUDIND REMARKS

This work accomplished a preliminary optimization study of a fluidized-bed boiler using a comprehensive mathematical simulator. It was based on two parameters: the number of tubes in the bed section and the air excess, while the fixed-carbon conversion factor and the boiler efficiency were chosen as two distinct optimization objectives. Results showed that high carbon conversions do not necessarily lead to elevated boiler efficiencies. The search for optimum operational conditions is a rather complex task since the driving parameters have mutual influences. For example, in order to achieve good boiler performances, one should take into account not only the effects related to the number of tubes in the bed section and air excess, but also those related to the bubble diameter and the bed average temperature. In such context, a reliable comprehensive mathematical simulator plays a major role.

Acknowledgements

The authors are grateful to FAPESP - Fundação de Amparo à Pesquisa do Estado de São Paulo - for their financial support to the research project (process no. 98/02891-8) to which this study belongs.

REFERENCES

Babcock & Wilcox, 1976, EPRI FP-308, vol. 2.

- de Souza-Santos, M. L., 1987, Modeling and Simulation of Fluidized-Bed Boilers and Gasifiers for Carbonaceous Solids, Ph.D. Thesis, University of Sheffield, Department of Chemical Engineering and Fuel Technology, England, United Kingdom.
- de Souza-Santos, M. L., 1989, Comprehensive Modeling and Simulation of Fluidized-Bed Boilers and Gasifiers, Fuel, vol. 68, pp. 1507-1521.
- de Souza-Santos, M. L., 1992a, Pressurized Fluidized-Bed Shale Hydroretorting Reactor Design; Considerations, Discussions and Approach through Comprehensive Simulation, IGT - Institute of Gas Technology, Chicago, Illinois, USA, May.
- de Souza-Santos, M. L., 1992b, Application of Comprehensive Simulation to Pressurized Fluidized-Bed Hydroretorting of Shale, Eastern Oil Shale Symposium, November 17-20, Lexington, Kentucky, USA.
- de Souza-Santos, M. L., 1992c, Modeling of Desulfurization Reactor, IGT Institute of Gas Technology, Chicago, Illinois, USA, February.

- de Souza-Santos, M. L., 1993a, Comprehensive Modeling and Simulation of Fluidized-Bed Reactors Used in Energy Generation Processes, Meeting on Energy Modeling Optimizing Information and Resources, June 7-8, Institute of Gas Technology, Chicago, USA.
- de Souza-Santos, M. L., 1993b, Simulation of Pressurized Fluidized-Bed Gasification of Biomass; Use of Comprehensive Model to Simulate the RENUGAS Process, IGT-Institute of Gas Technology, Chicago, Illinois, USA, February, Cliente: IGT.
- de Souza-Santos, M. L., 1994a, Application of Comprehensive Simulation to Pressurized Fluidized-Bed Hydroretorting of Shale, Fuel, vol. 73, no. 9, pp. 1459-1465.
- de Souza-Santos, M. L., 1994b, Application of Comprehensive Simulation of Fluidized-Bed Reactors to the Pressurized Gasification of Biomass, Proceedings of the 5th Thermal Sciences Brazilian Meeting, December 7-9, São Paulo, SP, Brazil, pp. 145-157.
- de Souza-Santos, M. L., 1995, Application of Comprehensive Simulation of Fluidized-Bed Reactors to the Pressurized Gasification of Biomass, J. of the Braz. Soc. Mechanical Sciences, vol. XVI, no. 4, pp. 376-383.
- de Souza-Santos, M. L., 1996a, Otimização Teórica e Testes Experimentais Preliminares de Gaseificação de RASF em Leito Fluidizado, IPT Instituto de Pesquisas Tecnológicas do Estado de São Paulo, Report no. 34.926/DME/AET, December.
- de Souza-Santos, M. L., 1996b, Sistema Gerador de Gás Quente de Leito Fluidizado para Utilização em Secagem de Espigas de Milho, IPT Instituto de Pesquisas Tecnológicas do Estado de São Paulo, Report no. 34.460/DME/AET, August.
- de Souza-Santos, M. L., 1997a, A Study on Pressurized Fluidized-Bed Gasification of Biomass through the Use of Comprehensive Simulation, Proceedings of the Fourth International Conference on Technologies and Combustion for a Clean Environment, July 7-10, Lisbon, Portugal, vol. 2, section 25.2, pp. 7-13.
- de Souza-Santos, M. L., 1997b, Search for Favorable Conditions of Atmospheric Fluidized-Bed Gasification of Sugar-Cane Bagasse through Comprehensive Simulation", XVI Congresso Brasileiro de Engenharia Mecânica, Dec. 8-12, Bauru, São Paulo, Brazil.
- de Souza-Santos, M. L., 1997c, Search for Favorable Conditions of Pressurized Fluidized-Bed Gasification of Sugar-Cane Bagasse through Comprehensive Simulation, XVI Congresso Brasileiro de Engenharia Mecânica, Dec. 8 -12, Bauru, São Paulo, Brazil.
- de Souza-Santos, M. L., 1997d, Assessment Study of an Alternative for Electric Power Generation Based on Biomass, 3° Simposio Nacional en Educación, Tecnología y Alternativas Energéticas, October 8-9, Instituto Pascual Bravao, Medellin, Colombia.
- de Souza-Santos, M. L., 1997e, Estudo de Viabilidade para Desenvolvimento de Sistema Alternativo de Geração Termoelétrica de Potência por Gaseificação de Biomassa e Turbina a Gás, IPT Instituto de Pesquisas Tecnológicas do Estado de São Paulo, Report no, 35.145/DEM/AET, March.
- de Souza-Santos, M. L., 1998, A Study on Pressurized Fluidized-Bed Gasification of Biomass through the Use of Comprehensive Simulation, in Combustion Technologies for a Clean Environment (chapter 4), Gordon and Breach Publishers, Amsterdam, Holland.
- de Souza-Santos, M. L., 1999, A Feasibility Study on an Alternative Power Generation System Based on Biomass Gasification/Gas Turbine Concept, Fuel, vol. 78, pp. 529-538.
- de Souza-Santos, M. L., Ushima, A. H., Guardani, R., 1992, Determination of Operational Conditions for the Reduction of CaSO₄ to CaS in a Fluidized Bed, IX Brazilian Congress on Chemical Engineering, September, Salvador, Bahia, Brazil.