Development and Validation of a 3-Dimensional CFB Furnace Model

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Abstract:

At Foster Wheeler, a three-dimensional CFB furnace model is essential part of knowledge development of CFB furnace process regarding solid mixing, combustion, emission formation and heat transfer. Results of laboratory and pilot scale phenomenon research are utilized in development of sub-models. Analyses of field-test results in industrial-scale CFB boilers including furnace profile measurements are simultaneously carried out with development of 3-dimensional process modeling, which provides a chain of knowledge that is utilized as feedback for phenomenon research. Knowledge gathered by model validation studies and up-to-date parameter databases are utilized in performance prediction and design development of CFB boiler furnaces. This paper reports recent development steps related to modeling of combustion and formation of char and volatiles of various fuel types in CFB conditions. Also a new model for predicting the formation of nitrogen oxides is presented. Validation of mixing and combustion parameters for solids and gases are based on test balances at several large-scale CFB boilers combusting coal, peat and bio-fuels. Field-tests including lateral and vertical furnace profile measurements and characterization of solid materials provides a window for characterization of fuel specific mixing and combustion behavior in CFB furnace at different loads and operation conditions. Measured horizontal gas profiles are projection of balance between fuel mixing and reactions at lower part of furnace and are used together with both lateral temperature profiles at bed and upper parts of furnace for determination of solid mixing and combustion model parameters. Modeling of char and volatile based formation of NO profiles is followed by analysis of oxidizing and reducing regions formed due lower furnace design and mixing characteristics of fuel and combustion airs effecting to formation of NO furnace profile by reduction and volatile-nitrogen reactions. This paper presents CFB process analysis focused on combustion and NO profiles in pilot and industrial scale bituminous coal combustion.

Keywords 3-dimensional CFB model, furnace profiles, combustion, NO_X model

INTRODUCTION

The complexity of the CFB furnace process and the large dimensions of commercial CFB units set challenges for the 3-dimensional CFB furnace process modeling. Generally agreement exists that development of microscopic CFD modeling approaches suffers from both lack and difficulty of having relevant measured validation data from industrial-scale CFB furnace operation and long calculation times. Another approach is macroscopic modeling with empirical or semi-empirical expressions to solve the furnace process with a coarser mesh and longer time step or in steady-state conditions. The model used for the present work solves the three-dimensional CFB furnace process in steady state condition using semi-empirical approach and it is based on original code developed in 1989 (Hyppänen et al, 1991).

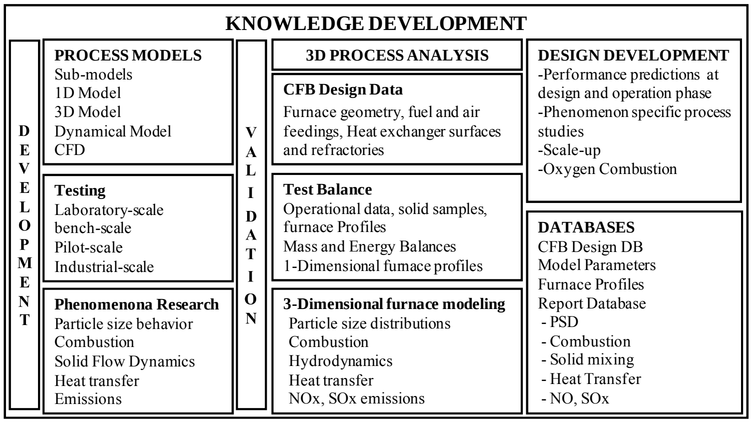

Fig. 1 CFB process knowledge development

The 3-dimensional CFB furnace model is a CFB process expert tool providing framework for testing and validating developed sub-models and theories, e.g. considering combustion and NO formation, against pilot and industrial scale test data with systematic approach. Knowledge gathered with CFB process analyses including 3D furnace modeling supports both CFB design development and operation phase optimization aspects (Fig. 1).

MODEL DESCRIPTION

The model solves the three-dimensional CFB furnace process in steady-state conditions using semi-empirical approach. Fig. 2 presents the general structure of the model. The different boundary conditions are defined directly from a boiler design tool. Furnace volume is discretized by hexahedral control volumes with typical cell dimensions 0.2...0.5 m and first-order upwind scheme is used as a solution method. Typical calculation time for grid sizes of 200 000 cells is 10-20 minutes for first calculation and less than 5 minutes for consequent calculations with minor modifications. The geometry and the location of the inlets and outlets are modeled as true as possible, given the limited density of the calculation mesh. Balance equations are defined for mass, momentum, species and energy for gas and solid phases. Empirical correlations govern various phenomena: solid concentration of different solids (char, ash, sand, limestone – all divided to six particle size fractions), mixing of solid and gaseous species by diffusion/dispersion, reaction rates, comminution and heat transfer. The validation of empirical correlations is based mostly on field tests at commercial units. The model principle and previous validation studies have been presented in earlier articles (Myöhänen et al.).

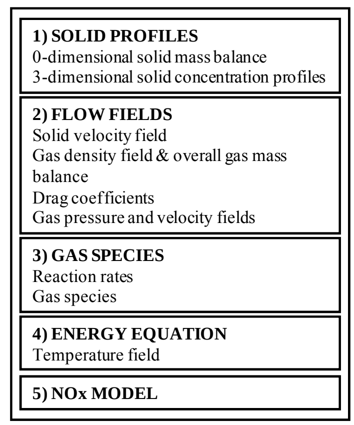

Fig. 2 General model structure

Combustion and NO_X Models

Fig. 3 presents the principle of the fuel combustion model. Fuel particle is divided to char, volatiles, ash and moisture according to standard proximate analysis and to six particle size fractions in order to enable simulation of comminution and effects of particle size on reactions and flow dynamics. The elemental composition of char and volatiles are determined based on ultimate analyses of char and fuel of different fuel types. Volatile release rate is defined by correlation counting particle diameter and by coefficient depending on fuel type and temperature.

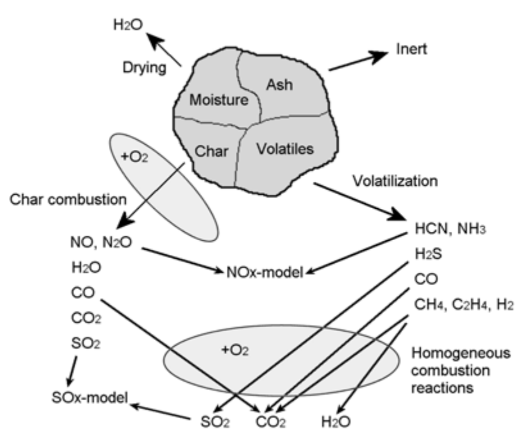

Fig. 3 Solid fuel combustion model

The formation of different gaseous species from devolatilization is modeled according to following principles: 1) nitrogen forms hydrogen cyanide (HCN) and ammonia (NH_3), 2) sulfur forms hydrogen sulfide (H_2S), 3) Oxygen forms carbon monoxide (CO) limited by the amount of carbon left, 4) excess oxygen forms molecular oxygen (O_2) and 5) remaining carbon and hydrogen form methane (CH_4), ethylene (C_2H_4), hydrogen (H_2) and free carbon (free-C) based on the molar ratio of H/C.

The split between the HCN and NH_3 is fuel specific and a correlation based on fuel O/C-ratio is used. The NO precursors (HCN and NH_3) are handled according to NO_x model reactions and the other formed gas species are combusted in the presence of oxygen according to combustion reactions (Table 1).

The local reaction rate is depending on the local concentrations of combusting gas, oxygen, water vapor, excess pressure and temperature. The reaction rate is calculated with a generic expression having empirical parameters. Reaction rate for carbon monoxide is

Table 1 Combustion and NO_X reactions

No.	REACTION
	Volatiles
1	$H_2S + 1.5\ O_2 \rightarrow SO_2 + H_2O$
2	$CO + 0.5\ O_2 \rightarrow CO_2$
3	$CH_4 + 0.5\ O_2 \rightarrow CO + 2\ H_2$
4	$C_2H_4 + 0.5\ O_2 \rightarrow CH_4 + CO$
5	$H_2 + 0.5\ O_2 \rightarrow H_2O$
6	$C_{free} + 0.5\ O_2 \rightarrow CO$
	Char
7	$C_{char} + (1-0.5\gamma)O_2 \rightarrow \gamma CO + (1-\gamma)CO_2$
8	$S_{char} + O_2 \rightarrow SO_2$
9	$H_{char} + 0.25\ O_2 \rightarrow 0.5\ H_2O$
	NOx Reaction (incl. catalysts)
R1	$HCN + O_2 \rightarrow NH_3$
R4	$HCN + O_2 + NO \rightarrow N_2O$
R5	$2\ HCN + O_2 \rightarrow N_2O$
R10	$NH_3 + O_2 \rightarrow NO$
R11	$NH_3 + O_2 + CaO \rightarrow NO$
R12	$NH_3 + O_2 + Char \rightarrow NO$
R13	$NH_3 + NO \rightarrow N_2$
R16	$N_{char} + O_2 \rightarrow NO$
R17	$2\ N_{char} + O_2 \rightarrow N_2O$
R18	$N_{char} + O_2 + NO \rightarrow N_2O$
R19	$NO + Char \rightarrow N_2$
R20	$NO + CO + CaO \rightarrow N_2$
R22	$N_2O \rightarrow N_2$
R23	$N_2O + CaO \rightarrow N_2$

$$R'''_{CO} = k_{CO}\,[CO]^{a_{CO}}\,[O_2]^{b_{CO}}\,[H_2O]^{c_{CO}} \left(\frac{p}{p_0}\right)^{p_{CO}} e^{-E_{CO}/RT} \quad . \qquad (1)$$

The char consists of C, H, S and N. The parameter γ in Table 1 (7) controls the CO/CO_2-ratio of carbon combustion. During combustion of char, the nitrogen forms NO and N_2O according to NO_x model. The other elements burn according to reactions in Table 1.

The NO_x reactions are solved after solution of the main furnace process. Fig. 4 presents the reactions paths of the current 3D CFB furnace NO_x model. The development of the new NO_x model for 3D-model is based on Foster Wheeler's 1D NO_x model. In the 1D model, NO_x reaction rate parameters have been empirically set by utilizing data and knowledge from test balances carried out at Foster Wheeler's commercial CFB units. The new NO_x model replaces the earlier model presented by Tsuo et al. (1995).

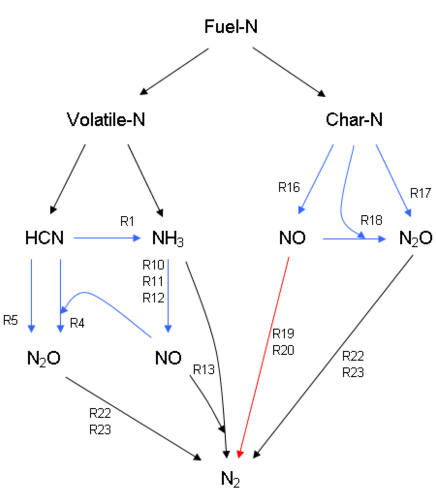

Fig. 4 NO_X reaction paths

VALIDATION

Scope and principles

Foundation of current 3D model validation concept is based on horizontal CFB furnace gas and temperature profile measurements together with mass and energy balance back-calculations with 1D CFB furnace model - validated with hundreds of test balances - providing for example fractional semi-empiric solid and char density profiles and solid comminuting characteristics.

The validation scope of the 3-dimensional CFB furnace model considering specifically lateral mixing based on horizontal furnace profile measurements consists of eight large-scale coal combusting CFB boilers and several peat, wood, biomass and waste fired CFB boilers. Bituminous coal combustion characteristics have been most extensively researched and range of validations cover capacities up to 370MW$_{th}$ and furnace depths of over 10m. Validations cover different operation conditions with full and lower load operation - unbalancing tests, air staging tests and co-combustion tests. Char and volatile release profiles with consequent combustion gas profiles are mainly determined by balance between fuel reactivity and mixing within constrains given by furnace design: anthracite tend to form even horizontal gas and temperature profile, lignite forms reductive zones above fuel feedings and combustion behavior of bituminous coal is between of those.

Horizontal shape and concentration level of oxygen, carbon monoxide and carbon dioxide is adjusted in 3D model validation calculations to correspond results of furnace profile measurements with combustion and solid mixing related validation parameters. Main validation parameters regarding combustion are char reaction rate, volatile release rate and CO reaction rate coefficient, which also consists micro-scale mixing limitation to reaction kinetics. Fractional char and volatile release profiles are formed according to relation of fuel mixing rate and reaction rate. Dispersion of fuel is defined with fractional char density related dispersion coefficients. Shape and level of vertical and horizontal temperature profiles are adjusted with model parameters affecting to solid mixing by fractional solid dispersion coefficients and by estimating heat flux profile with internal circulation model parameters and heat transfer coefficients.

Fig. 5 presents validation parameters effecting to char mixing and reactivity for bituminous coals. Recently also several combustion test periods executed at pilot-scale CFB test rig have been analyzed. 3D furnace model analysis of bituminous coal combustion pilot and industrial scale test balances aiming both to model validation and detailed process characterization are here presented.

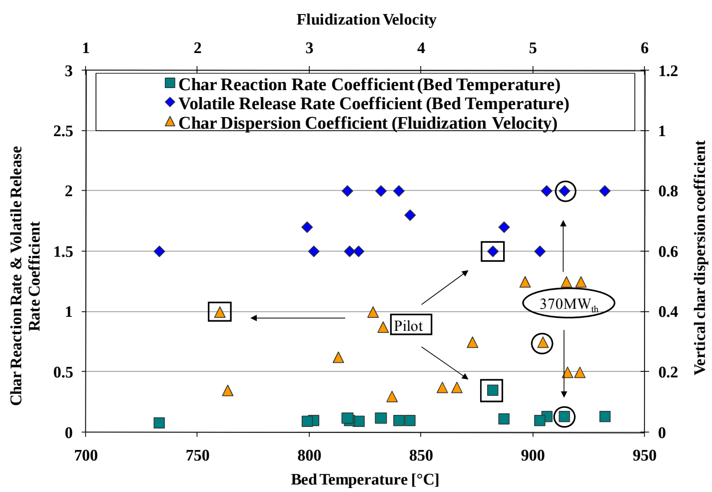

Fig. 5 Validated fuel dispersion (fluidization) and reactivity (temperature) parameters for bituminous coals.

Table 2 Operational Conditions

Fuel	**VTT Pilot** Bit. Coal	**370MW$_{th}$ CFB** Bit. Coal	**Operational Conditions**	**VTT Pilot**	**370MW$_{th}$ CFB**
Proximate analysis			Furnace		
Moisture, w-%	9.5	20	Fluidization velocity, m/s	2.3	5.2
Ash (815C), w-%	13.8	5.5	Grid air ratio, %	60	62
Volatile content, w-%	30.9	42.8	Temperature: bed, °C	882	932
Ultimate analysis			Solid density exit,kg/m^3	2.1	2.4
C, w-%	72.9	69.7	Bed pressure, kPa	2.07	5.3
H, w-%	4.29	5.0	Stack		
N, w-%	1.27	1.33	NO, ppm-dry	135	49
S, w-%	0.78	0.92	CO, ppm-dry	806	79
O, w-%	6.94	17.55	O2, %-dry	4.8	2.7
LHV-dry, MJ/kg	28.6	26.9			
Fuel size, D50	<0.5mm	1.6			

Pilot-scale CFB process analysis

VTT CFB pilot reactor (50 kW) described in detail in (Tourunen et al., 2008) is equipped with several separately controlled electrically heated and water/air cooled zones and three secondary air levels providing operation flexibility for controlling load and vertical oxygen and temperature levels independently.

Operational conditions of analyzed bituminous coal test balance are shown in Table 2. CFB Pilot reactor having 8 m riser height and 167 mm inner diameter was operated with 60% primary air ratio, 882°C bed temperature and 2.3m/s fluidization velocity. 3D-modeling approach for solid behavior characterization includes determination of both fractional solid and char density profiles. Total solid density profile is adjusted according to measured vertical pressure profile similarly to large-scale CFB boilers. Total solid loading was 4.3kg with solid density of 2.1kg/m^3 at dilute zone of reactor and 470kg/m3 at dense bed area. Char density of 0.2kg/m^3 was measured from dense bed area and 0.003kg/m^3 from upper dilute zone of reactor. As a part of char mixing and combustion analysis modeled fractional char density profiles are compared and fitted with measurements as shown in Fig. 6b. Char and volatile combustion profile, solid mixing behavior and heating/cooling profile of furnace define the temperature profile (Fig. 6a) of reactor.

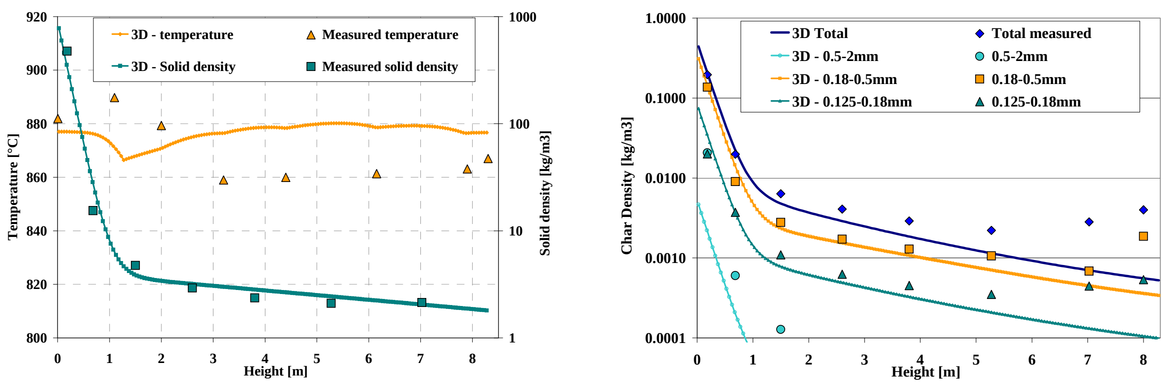

Fig. 6 (a) Temperature and solid density profiles (b) Fractional char profiles

Fig. 7 shows comparison of measured and modeled vertical combustion gas profiles and followed NO formation analysis with profile measurements of nitrogen compounds and NO model. Preliminary fit for NO_X model parameters used earlier in NO_X modelling of large-scale CFB furnace was here done based on experiments focused on effect of temperature and oxygen level to NO formation (Tourunen et al., 2008). In future empirical NO_X model parameter study combined to bench and pilot scale testing is required for further development of NO_X prediction capability.

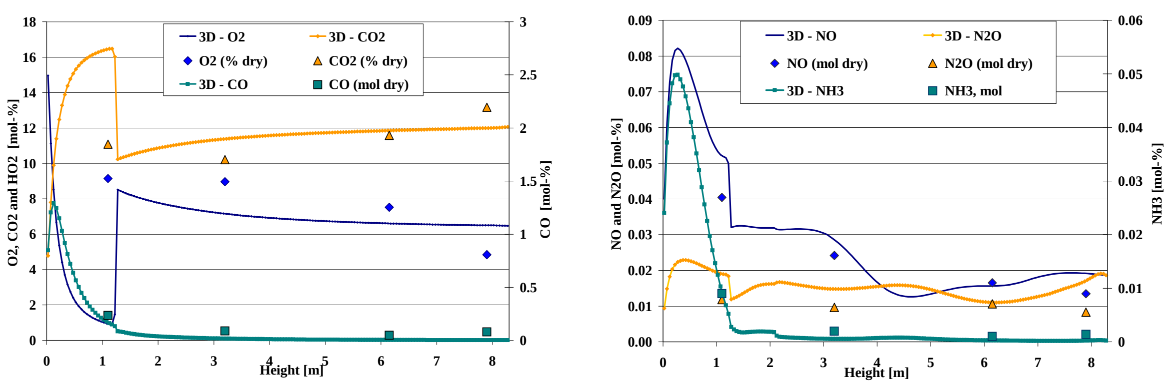

Fig. 7 Combustion (a) and NO (b) modeling of bituminous coal combustion at CFB Pilot

Stabilization of N-compound concentrations as well as combustion gas concentrations is both measured and modeled at upper parts of reactor, while conditions in dense bed area and in influence of secondary air mixing and reaction zone are mainly determining combustion and nitrogen chemistry related reaction rates, thus determining the levels of gas compound concentrations at upper part of reactor. Behavior is analogous for larger scale CFB furnaces and in future profiles are measured also at dense bed area.

Bituminous Coal Combustion in a Large-scale CFB Boiler

Results of 3D furnace model validation analysis of one bituminous coal test balance in 370MW$_{th}$ CFB boiler are presented. Investigated CFB furnace has 40.5m height and 15.9m x 7.8m cross-section with six fuel feedings located at two opposite walls and 24 secondary air nozzles at 2.5m above grid. CFB boiler is operated with 100% load, 62% grid-to-total air-ratio, 5.2m/s fluidization velocity and 932°C bed temperature. Combusted coal has relatively high volatile, 43% on dry basis, and low ash content, 5.5% on dry basis. Main operation parameters and fuel analysis are summarized in table 2.

Furnace profile measurements show increased CO and low O_2 concentrations above fuel feedings at horizontal cross-section 10m above grid, while adjacent measurements above related secondary air nozzles shows low CO and respectively high O_2 concentrations. Similar combustion gas profile shapes and concentration levels were achieved by 3D furnace model process and validation analysis including predicting fractional char mixing and reactivity, volatile release profiles and both mixing and reactivity of gases species. High CO concentrations are modeled in front of fuel feedings from dense bed area to SA nozzle level. Secondary air fed to this region of intensive volatile release combusts CO at SA jet influence area and further CO reactions controlled by macro and micro scale gas mixing taking place in upper parts of furnace reduce CO concentration with much lower gradient.

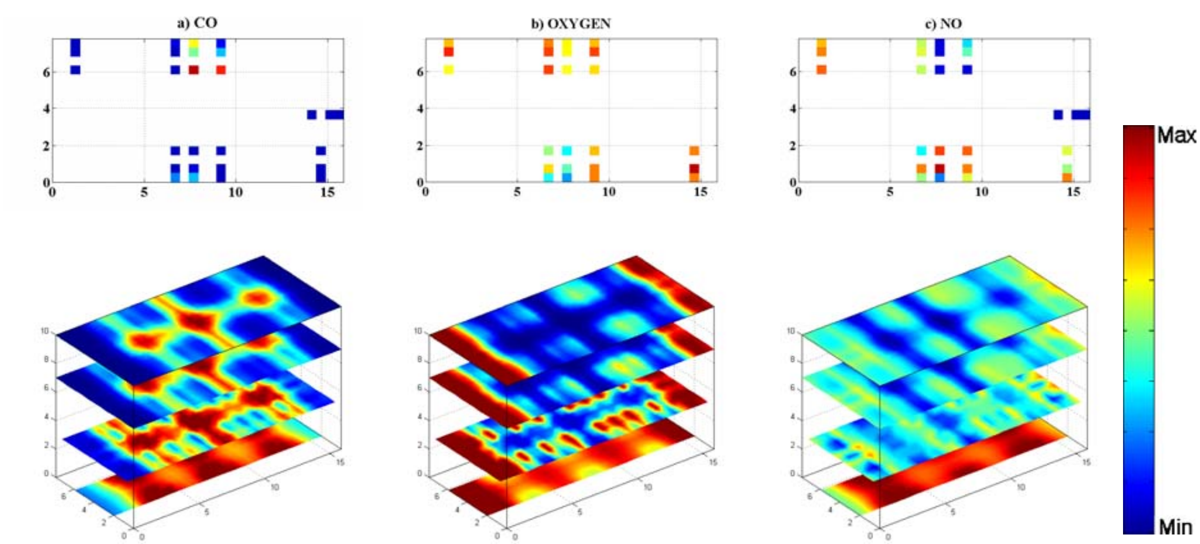

Fig. 8 Measured (10m) and modeled a) CO, b) oxygen and c) NO concentration profiles

Basis for NO_X model post-calculation is provided by predicted char density, oxygen, carbon monoxide and temperature profiles. Fig.6 presents comparison of measured horizontal profiles and modeled formation of NO concentration profile in lower furnace. Similar NO profile shape is achieved with NO_X model as measured in horizontal cross-section 10m above grid. High NO concentrations are both modeled and measured above SA nozzles next to fuel feedings, while reductive char and CO rich conditions above fuel feedings resulted lower modeled NO concentrations shown also by the measurements.

CONCLUSIONS

3-dimensional furnace model is part of overall CFB process know-how development carried out by testing, modeling and analyzing in different scales: from laboratory-scale analyses to field tests at large-scale industrial CFB boilers. Sub-models are continuously further developed, and here principle of combustion model and updated NO_X model was presented. Reactions and parameters of implemented NO_X model are based on 1-dimensional NO_X model that has been validated against hundreds of test balances carried out in CFB boilers firing different types of fuels.

3D CFB furnace model is validated against several steady-state test balances carried out in industrial-scale CFB boilers combusting different types of coals and biomass regarding combustion and solid mixing characteristics. Horizontal furnace profile measurements being part of the process analysis have provided information on lateral mixing, which is one of the key factors concerning scale-up of CFB boilers. Additionally presented NO_X model has been utilized for NO profile formation analyses of several coal-fired CFB boiler furnaces. Recently results of pilot-scale experiments are utilized in 3D furnace model validation and pilot characterization. Focus has been on formation of combustion and NO profiles due fuel and operating condition specific char and volatile profiles.

Vertical and lateral combustion gas profiles and temperature profiles can be predicted also for design phase CFB boiler furnaces. Prediction of NO formation requires pre-modeled 3-dimensional char density, volatile release and temperature profiles and combustion gas profile with its reductive and oxidizing regions to be comparable with real process conditions. With current NO_X model formation of volatile and char based nitrogen compounds can be simulated and comparison with horizontal gas profile measurements in case of bituminous coal combustion in large-scale CFB boiler showed that similar NO profile shape can be achieved by NO_X model implemented to 3D CFB furnace model.

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