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Further improvement of fluidized bed models by incorporating zone method with Aspen Plus interface

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Abstract

While providing a fast and accurate tool of simulating fluidized beds, the major limitation of classical zero-dimensional ideal reactor models used in process simulators, such as models built into commercial software (e.g. Aspen Plus®), has been the difficulties of involving thermal reciprocity between each reactor model and incorporating heat absorption by the water wall and super-heaters which is usually specified as model inputs rather than predicted by the models themselves. This aspect is of particular importance to the geometry design and evaluation of operating conditions and flexibility of fluidized beds. This paper proposes a novel modelling approach to resolve this limitation by incorporating an external model that marries the advantages of zone method and Aspen Plus in a robust manner. The improved model has a relatively modest computing demand and hence may be incorporated feasibly into dynamic simulations of a whole power plant.

1. Introduction

Circulating Fluidized Bed (CFB) technology has been developed and served as effective method for burning solid fuels for many industrial applications since the 1980s, such as coal combustion, due to its inherent advantages over conventional combustion method like fuel flexibility, high combustion intensity, and low emissions [1]. Although technical knowledge about the design and operation of CFB is widely available for pilot plant and large scale units [2], few have conducted modelling of the whole CFB power plant and hence little is known about its dynamic performance and operational flexibility [3]. This might be due to the fact that the combustion process occurring in a CFB boiler involves complex phenomena like

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chemical reactions, heat and mass transfer, particle reduction due to combustion and it may also lie in the shortage of effective modelling approaches.

Nomenclature

Abbreviations

ABFBC	Atmospheric Bubbling Fluidized-Bed Combustor
CFB	Circulating Fluidized Bed
CPFD	Computational Particle Fluid Dynamics
DFAs	Directed Flux Areas
MCRT	Monte-Carlo based Ray-Tracing
TEAs	Total Exchange Areas

Symbols

A_i	area of the i-th surface zone	m^2
$\overline{G_1G_J}, \overline{G_1S_J}, \overline{S_1G_J}, \overline{S_1S_J}$	directed flux areas	m^2
K_i	extinction coefficient of gas zone i	m^{-1}
$\dot{m}$	mass flow rate	$kg\ s^{-1}$
$\dot{q}_{conv,i}$	heat convection term of surface zone i	$W\ m^{-2}$
$\dot{Q}_{conv,i}$	heat convection term of gas zone i	W
$\dot{Q}_{enth,i}$	enthalpy transport term of gas zone i	W
$\dot{Q}_{s,i}$	net radiation from the surface zone i	W
$\dot{Q}_{g,i}$	net radiation absorbed by the gas zone i	W
$T_{g,i\ or\ j}$	temperature of gas zone i or j	K
$T_{s,\ i\ or\ j}$	temperature of surface zone i or j	K
V_i	volume of gas zone i	m^3
σ	Stefan-Boltzmann constant (5.6687×10^{-8})	$W\ m^{-2}\ K^{-4}$

CFB modelling has been implemented using commercial software for a long time, such as Aspen Plus® [4-7] and Computational Particle Fluid Dynamics (CPFD)® [8-9]. Although the advancement in Aspen Plus has made time-dependent dynamic simulation, prediction and control of CFB combustion processes in real time possible, the major limitation is that classical zero-dimensional ideal reactor models used in Aspen Plus has been the difficulties of involving thermal reciprocity between each reactor model and incorporating heat absorption by the water wall and super-heaters which is usually specified as model inputs rather than predicted by the models themselves. This aspect is of particular importance to the geometry design and the evaluation of operating conditions and flexibility of fluidized beds. On the other hand, although CPFD is widely used to simulate combustion systems and can predict the detailed local heat and mass transfer information available for the entire computational domain, it often takes several days if not weeks to provide useful results for large industrial cases. Therefore, CPFD models are unlikely for being incorporated into dynamic simulations and used to study the starting up and shutting down a plant, changes of conditions during a reaction, holdups, thermal changes and more.

In fluidized beds, the combustion efficiency depends on the heat recovered in the freeboard region, where the dominant component of heat transfer is radiation [10]. Therefore, the modelling of the radiative heat transfer in such systems necessitates an accurate knowledge of the radiative analysis. This paper aims to frame a modelling approach that can compromise the above limitations existing in CFB modelling, but not limited to CFB modelling, and involve radiative analysis by incorporating an external model that marries the advantages of zone method [11] and Aspen Plus simulation in a robust manner. The improved model is

expected to have a relatively modest computing demand and hence feasible to be incorporated into dynamic simulations of a whole CFB power plant.

2. Modelling object

A 0.3MW Atmospheric Bubbling Fluidized-Bed Combustor (ABFBC) test rig is used as the simulation object in this work, as shown in Figure 1 [12]. The main body of the test rig is the modular combustor formed by five modules of internal cross section of 0.45×0.45 m and 1 m height. The inner walls of the modules are refractory lined and insulated. The first and fifth modules refer to the bed and cooler, respectively, and the ones between them are the freeboard modules. There exist two cooling surfaces in the modular combustor, as shown in Figure 1, providing 0.35 m^2 and 4.3 m^2 of cooling surfaces, respectively.
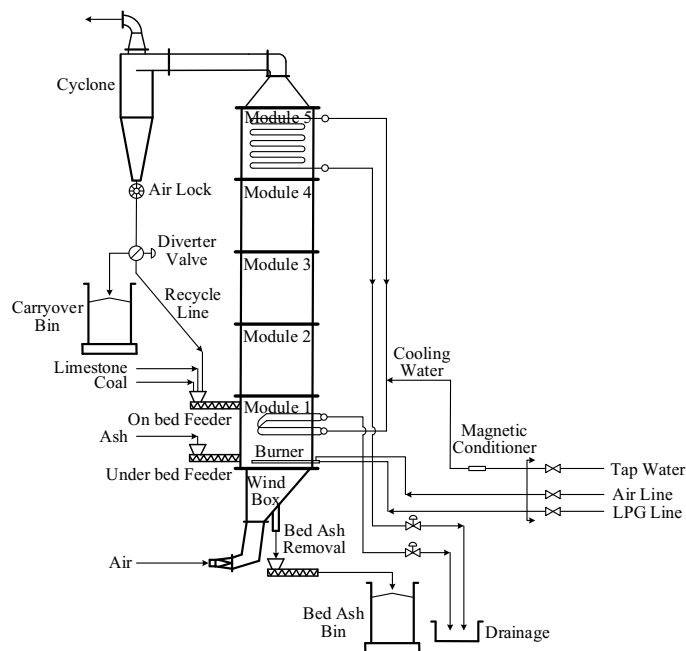

Fig. 1. Schematic of the 0.3 MW ABFBC test rig

3. Modelling approaches

The previous work of *Sotudeh-Gharehaagh et al.* [4] had described in details the implementation of Aspen Plus reactor modules [13] for CFB modelling and hence need not to be repeated here. This paper mainly focuses on the further improvement of the fluidized bed models within the framework of Aspen Plus by incorporating a rigorous radiation sub-model based on the zone method of radiation analysis.

According to the zone method, the relatively simply geometry of the ABFBC is split into a finite number of isothermal volume and surface zones along the height of the freeboard region, as shown in Figure 2. The bottom and the top surfaces including cooling tubes are approximated by equivalent black and gray surface respectively, for modelling purpose. The assumption of plug flow is applied to the flow pattern, and this is reasonable since the flow pattern-led enthalpy transport is dominated in the longitudinal direction of the

fluidized bed. However, even more complicated zoning arrangement and flow pattern are also possible, see [14], which depend on the requirements of a specific problem. An energy balance is formulated for each zone taking into account radiation interchange between all volume and surface zones, the enthalpy transport, and the source term associated with convection [15]. Figure 3 shows the zone model incorporated Aspen Plus flow sheet for ABFBC modelling. RYield (Aspen Plus reactor) is used to model the devolatilization process by specifying the yield distribution vector via an In-Line Fortran Calculator 1 (Aspen Plus calculator block) according to the coal ultimate analysis; RStoic (Aspen Plus reactor) is used to model volatile combustion process by specifying the fractional conversion of key components via an In-Line Fortran Calculator 2; the mean axial voidage in a certain interval between different heights of the combustor is calculated via an In-Line Fortran Calculator 3; char combustion above bed is implemented using a set of RCSTRs (1 to 6 in this case, Aspen Plus reactor) with the user defined kinetics – USRKIN.f (Aspen Plus Subroutine). In the simulation, the RCSTR block temperatures are recalculated by the zone model based on the retrieved enthalpy flows at each iteration to get a new value as the initial value at the next iteration until the convergent tolerance is satisfied.
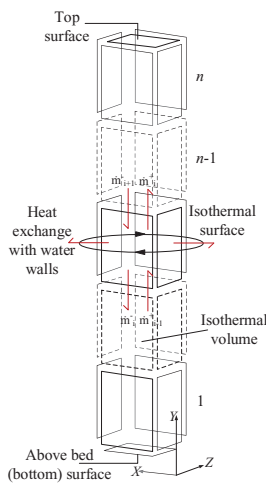

Figure 2 Illustration of zone method applied in the freeboard region of ABFBC
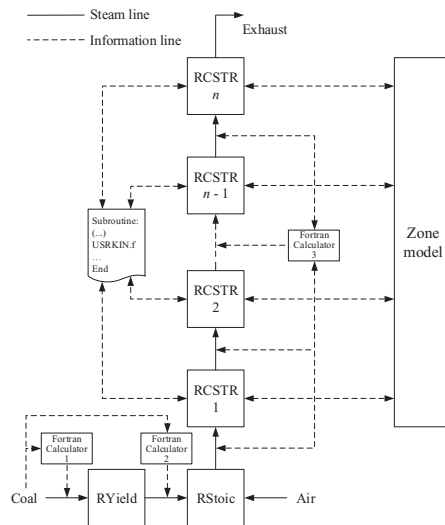

Figure 3 Zone model incorporated Aspen Plus flow sheet for ABFBC modelling

The radiation term in the energy balance equations is written in terms of exchange factors known as Directed Flux Areas (DFAs) (denoted by $\overline{G_iG_j}, \overline{G_iS_j}, \overline{S_iG_j}, \overline{S_iS_j}$ for gas-gas, gas-surface, surface-gas, and surface-surface exchange respectively in *Eqs*. 1 and 2). The energy balances on all zones yield a set of simultaneous non-linear equations which can be solved to determine the temperature and heat flux at each zone.

For a system of N volume zones and M surface zones, the following energy balances can be written.

$$\dot{Q}_{g,i} = \sum_{j=1}^{N} \overline{G_iG_j}\sigma T_{g,j}^4 + \sum_{j=1}^{M} \overline{G_iS_j}\,\sigma T_{s,j}^4 - 4K_iV_i\sigma T_{g,i}^4 - \dot{Q}_{\text{conv},i} + \dot{Q}_{\text{enth},i}, \qquad (Eq.\ 1)$$

$$\dot{Q}_{s,i} = \sum_{j=1}^{M} \overline{S_iS_j}\sigma T_j^4 + \sum_{j=1}^{N} \overline{S_iG_j}\,\sigma T_{g,j}^4 - A_i\epsilon_i\sigma T_i^4 + A_i\dot{q}_{\text{conv},i}. \qquad (Eq.\ 2)$$

For the i-th volume (gas) zone, $\dot{Q}_{g,i}$ represents the net rate of heat transfer to the volume (gas) zone; likewise, for the i-th surface zone, $\dot{Q}_{s,i}$ represents the net rate of heat transfer to the surface zone.

The DFAs in *Eq*. 1 – *Eq*. 2 are the function of Total Exchange Areas (TEAs). The TEAs in this study are calculated using an updated Monte-Carlo based Ray-Tracing (MCRT) algorithm [16] which is also capable of taking into account the individual obstacle geometry inside the computational domain of even more complicated applications. The radiative properties of the particle laden combustion gases are assumed to be uniform and constant throughout the freeboard region. Adiabatic condition is applied to the wall surfaces along the freeboard region, and $\dot{Q}_{s,i}$ therefore equals to zero in this case. The detailed boundary conditions and operating conditions are given in [17]. These data, together with retrieved enthalpy flow data in Figure 3, provide the input data that needs to be supplied to the zone model.

From a given boundary condition these *M+N* non-linear equations can be solved using the Newton-Raphson method [18]. This method provides an approach of computing successive approximations to the variables which converge towards the solution.

4. Results and discussion

The ABFBC during a steady state operation [17] was simulated in this work. The calculation took 0.67 second to get a converged solution after 8 iterations, and the maximum temperature difference between the values calculated by RCSTR blocks and zone model was less than 10^{-4} K. The measured and predicted thermal behaviours, including gas temperature profile and incident radiative heat fluxes, are shown in Figures 4 and 5, respectively. The gas temperature profiles are found to be in good agreement, but appreciable discrepancies are found in incident radiative heat fluxes at the locations close to the bed and the cooler. Further sensitivity study on the emissivity of the top and bottom surfaces showed that the discrepancies were not mainly attributed to the emissivity values specified to the equivalent surfaces. This might be due to the equivalent surfaces which do not really exist and the radiometer probes located at those heights are also affected by the cooling tubes. In addition, since the inner walls of the freeboard are refractory lined and insulated, heat losses are negligible. The wall temperatures of the freeboard are close to the adjacent gas temperatures during the steady state operation.
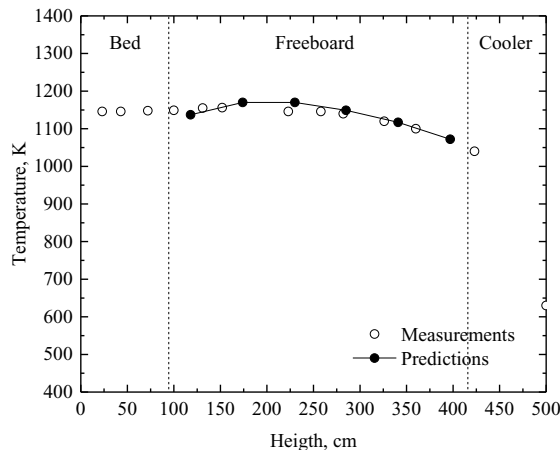

Figure 4 Measured and predicted gas temperature profiles along the height of combustor
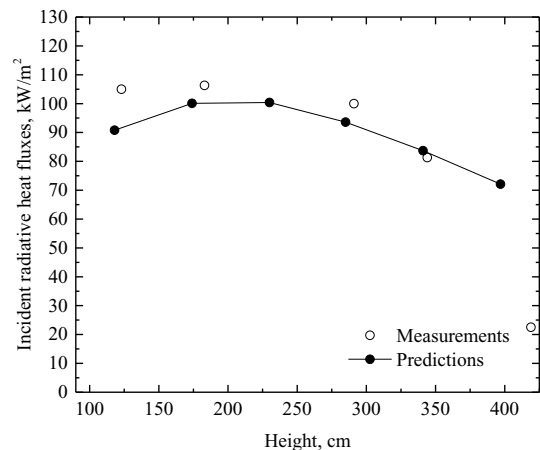
Figure 5 Measured and predicted incident radiative heat fluxes on freeboard side walls

The results above demonstrated that the improved fluidized bed model has a relatively modest computing demand so that it may be incorporated into dynamic simulations of a whole power plant. The implication of current work highlighted the existing limitation of sequential modular strategy in Aspen Plus, in that there is no thermal reciprocity within its modelling framework. By incorporating zone method with Aspen Plus interface in this work, the energy balance takes into account of radiation interchange between all volume and surface zones, the enthalpy transport, and the source term associated with convection. Although the improved model is one-dimensional in this case, the proposed modelling approach is equally applicable to two- and three-dimensional cases. For a multi-dimensional model, the enthalpy transport term needs to be expanded to include the flows in all relevant directions. The flow data may be provided from other physical models, like computational fluid dynamics isothermal simulations [14].

5. Conclusions

The further improvement is demonstrated in the current paper which highlights a novel modelling approach of fluidized beds to incorporate the classical zone method with Aspen Plus interface. A particular advantage of the improved model arises from the thermal reciprocity within a modules formed combustor derived from zone method which beaks the limitation of sequential modular strategy in Aspen Plus. The improved model has been validated by measurement data from a 0.3MW atmospheric bubbling fluidized-bed combustor test rig. Relatively modest computing demand and acceptable accuracy make it possible for the improved model to be incorporated into dynamic simulations of a whole power plant and then used to study the dynamic response performance and operation flexibility of the whole power plant.

Acknowledgements

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