CHAPTER 4

Numerical Simulation

This chapter gives the detail of numerical simulation in slag problem. The FactSage program and ANSYS Fluent were used in this work. The numerical modeling steps of the programs required for any given reaction mechanism are presented.

4.1 FactSage® Modeling

FactSage is the largest thermochemical package and database available for inorganic solid and slag in the field of computational thermochemistry. The Equilib module (thermodynamic application calculations) and Phase Diagram module (phase diagram calculations) are used to incorporate the FactSage Gibbs energy minimizer. Gibbs energy minimization techniques are characterized by the species molar amounts. The system systematically altered from an initial value to the lowest total Gibbs energy at a specified pressure and temperature. The total Gibbs energy for a phase at the constant of pressure and temperature was calculated by Eq. (4.1) (Eriksson and Konigsberger, 2008). In this study, the FactSage program version 6.4 (Figure 4.1) was supported by Energy Technology Innovation Initiative, the University of Leeds.

The program provides the ability to calculate and manipulate phase diagrams, established mainly in the field of complex chemical equilibrium and process simulations. It is used to supply insight into specific mineral interactions, slag formation and slag liquid temperatures of mineral compositions. The database can assist in the understanding, as well as predicting, what might happen with specific coal and mineral sources during the gasification or combustion processes.

$$G = \sum n_i (g^\circ_i + RTlnx_i + RTln\gamma_i) \quad (4.1)$$

Where n_i is a specie molar amount, R is the gas constant, T is the temperature. While ${g°}_i$ is the standard molar Gibbs energy, and $RTln\gamma_i$ is the partial molar excess Gibbs energy, which are in general pressure and temperature dependent and might also include magnetic contributions.

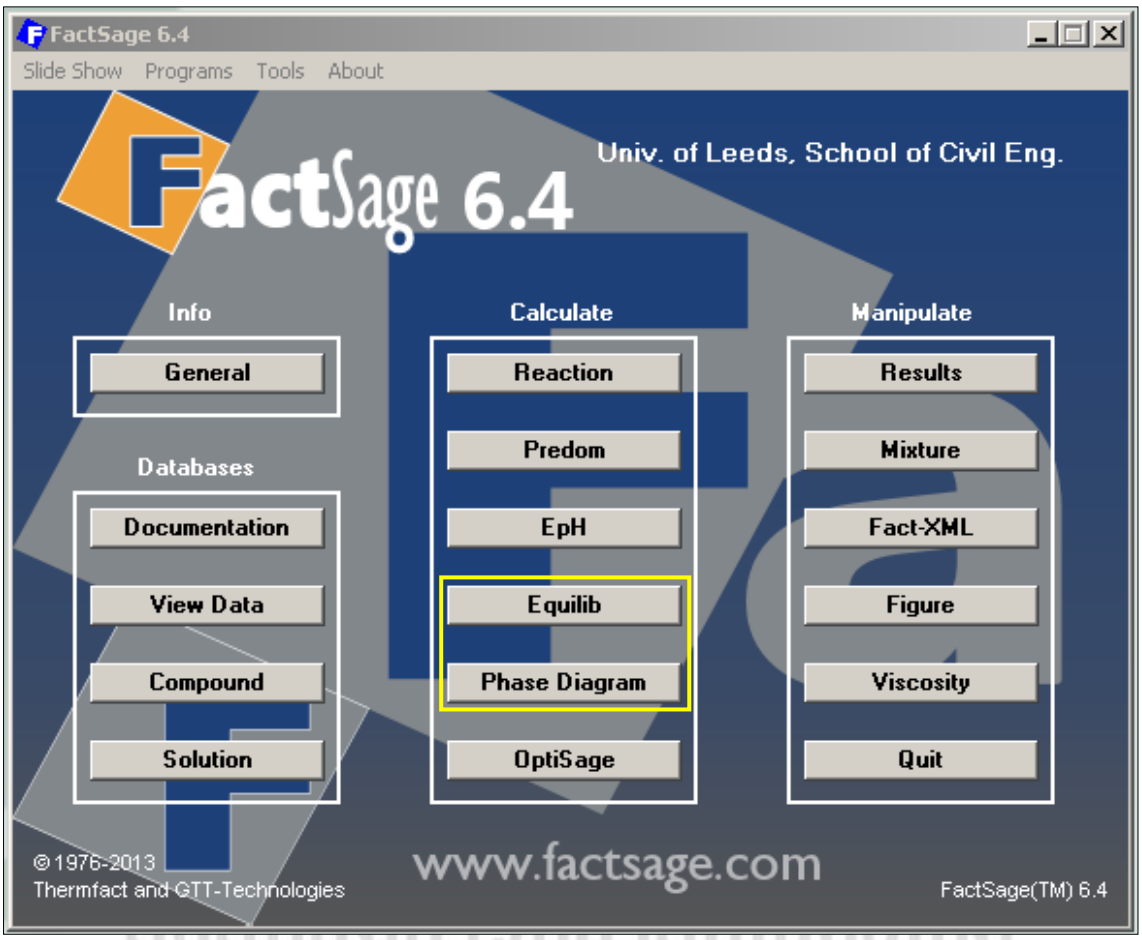

Figure 4.1 The FactSage program version 6.4

4.1.1 Equilib Module

The Equilib module performs complex equilibrium calculations for multicomponent, multiphase systems. The flow chart of steps is shown in Figure 4.2. The reactants are defined, the possible compound and solution products are selected, and the temperature and pressure conditions are set. The products (gas, liquid, solid, slag, etc.) are calculated and automatically presented at the end calculation (Bale et al., 2002; Bale et al., 2009;

Eriksson and Konigsberger, 2008). In this study, the calculations were performed under the oxidizing condition at 1-atm pressure with a FToxide database. The data of reactant (the mass of carbon, hydrogen, nitrogen, oxygen, and sulfur in coal, the mass of Na_2O, MgO, Al_2O_3, SiO_2, P_2O_5, SO_3, K_2O, TiO_2, Fe_2O_3, CaO, and MnO_2 in ash) was input in the FactSage Equilib module with 3% of access oxygen. The temperature range refered to the coal combustion in boiler furnace was specified as 800°C to 1600°C at 50°C intervals. This study focuses on the slag formation and the mineral composition of the slag-liquid portion at specific temperature.

4.1.2 Phase Diagram Module

The Phase diagram module was used to calculate, plot and edit the phase diagram sections where the axes can be various combinations of temperature, pressure, chemical composition, etc. Phase-equilibrium considered yields the lowest temperature at which the ash will be completely liquid (liquidus temperature) and the composition of solid and liquid phases at intermediate temperature (Huggins et al., 1981).

In this study, mass fractions of ash composition of SiO_2, Al_2O_3, CaO, Fe_2O_3 (oxidizing conditions), Na_2O, and MgO and temperature were input into the module. The solution database used was FToxid-SLAGA for pure solids products with a pressure 1 atm. The superimpose function in the Figure module was used for the interface with the phase diagram. All the steps are present by Figure 4.3. The composition point can be inserted to predict the ash fusion temperature. Initially, only the first three major components (SiO_2, Al_2O_3, and CaO) were considered for the ternary phase diagram. Subsequently, an additional component (chosen from Fe_2O_3, Na_2O, or MgO) was employed to simulate the quaternary phase diagram.

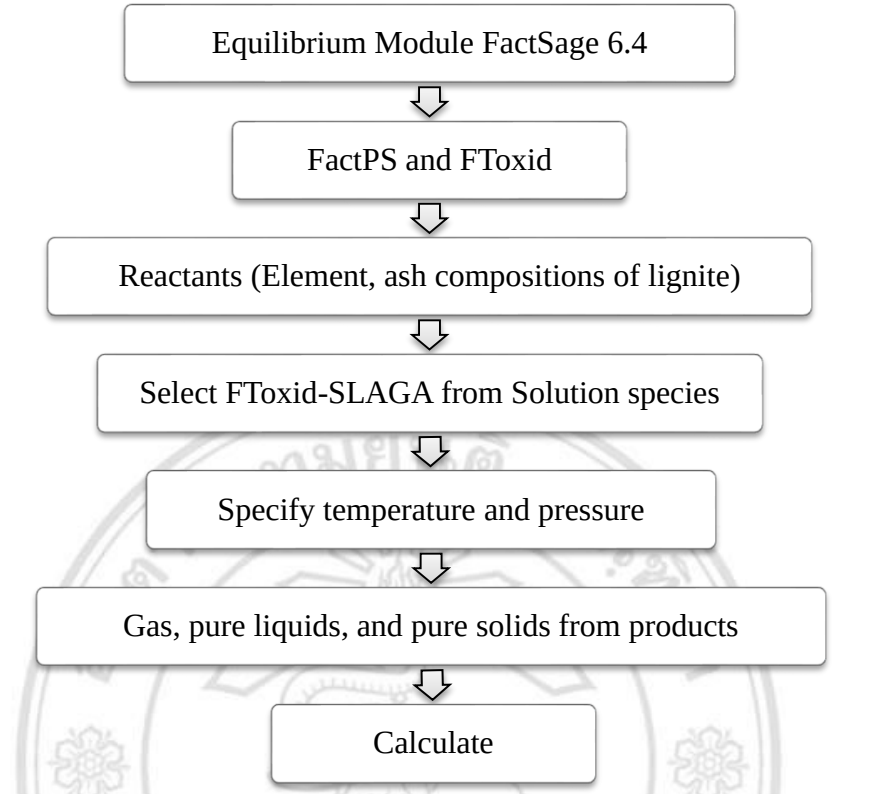

Figure 4.2 Flow chart of Equilib module simulation

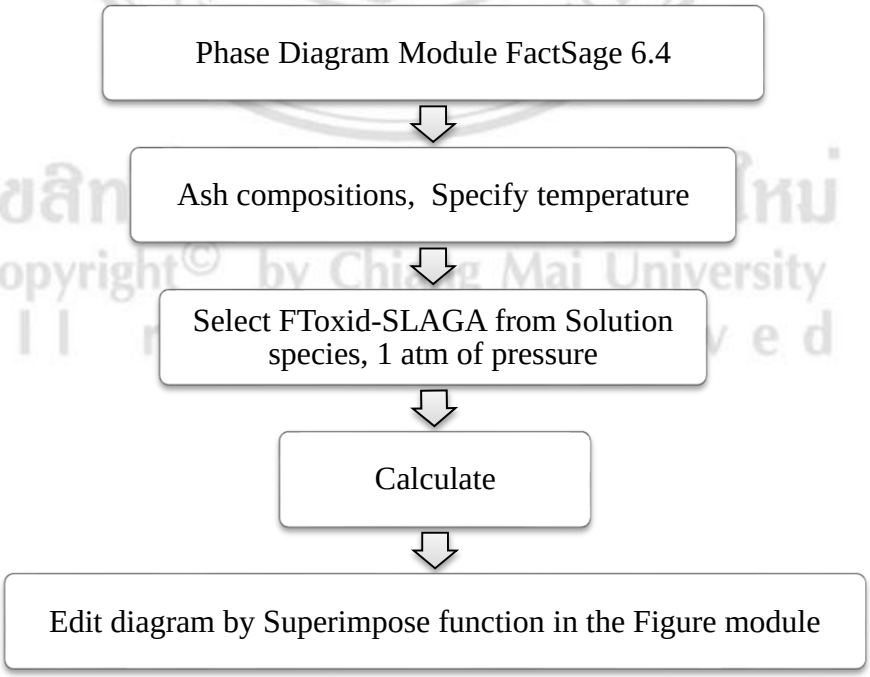

Figure 4.3 Flow chart of Phase Diagram module simulation

4.2 Computational Fluid Dynamic Modeling

In generally, coal combustion in CFD models have been used to solve the fluid flow, turbulence, particle trajectories, heat transfer, chemical reactions of the fuel, and the formation of pollutants (Backreedy et al., 1999). In this study, the FLUENT Version 13.0 was used to predict the temperature and flow distributions inside a boiler, and the wall heat flux to compare with the real operation (Figure 4.4). The results can be combined with the FactSage method to predict the deposition of the slag in the boiler furnace. Setting up a case required the geometry with grid that sufficiently describes the physical volume in the simulation.

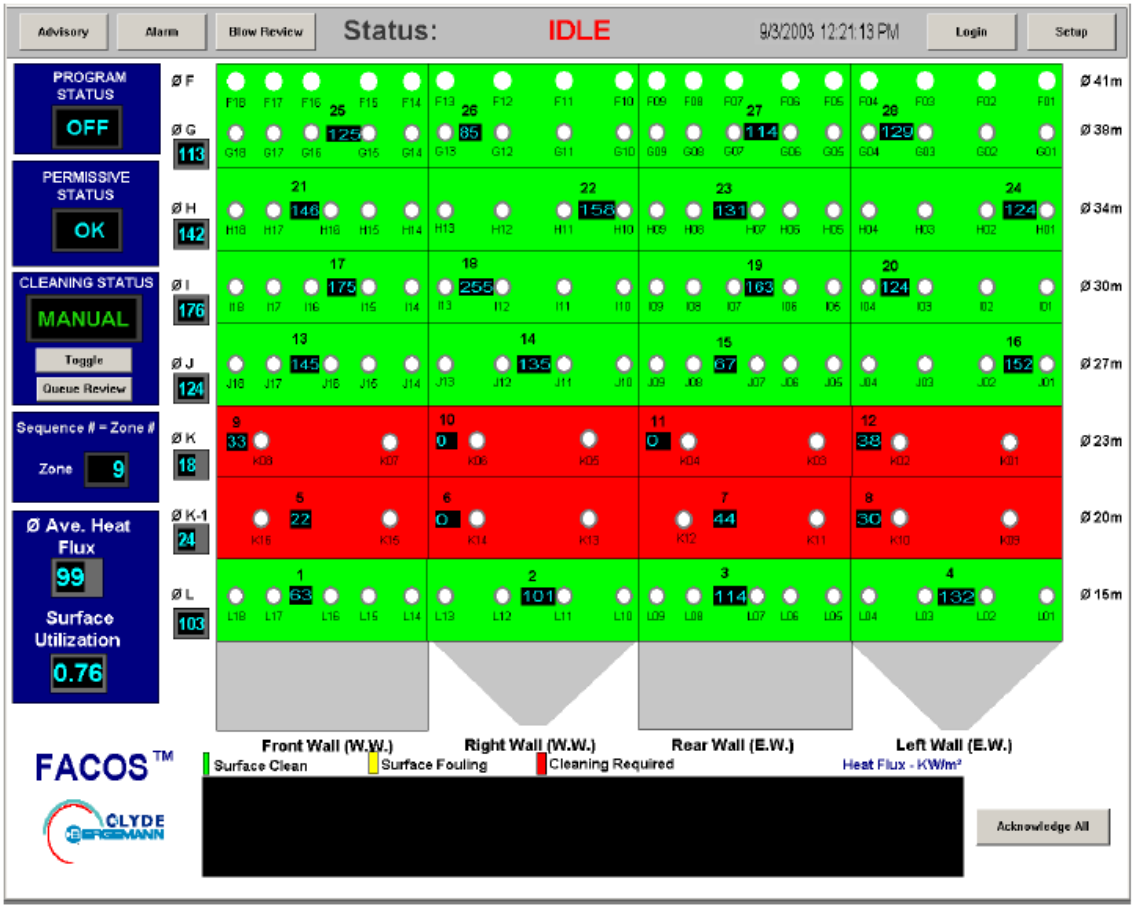

Figure 4.4 The measured of wall heat flux from FACOS system in Mae Moh power plant

In order to simulate coal combustion, the important steps is shown in Figure 4.5. The geometry and computational grid to represent the boiler furnace were generated and imported to FLUENT. The suitable sub-models and parameters were used to set up simulations in FLUENT 13.0 software, to set up the initialize and solution monitors, then the solution was run. The results are accepted when the solution is converged with accuracy. If not, the parameter or grid of solution was refined.

4.2.1 Geometry and Grid Generation

A Mae Moh furnace of 300 MW with a tangentially fired boiler was generated using a 3-D geometry in ICEM CFD. This is shown in Figure 4.6. The dimensions of furnace are 13.8 m. in width and 15.3 m. in depth. The geometry height from the lowest at the hopper to the highest at the Superheater and Reheater is 54.3 m. In the walls, there are 4 windboxs for 4 corners to generate fired ball in the tangential direction. There are 4 secondary air panels, 5 of the mixing of primary air and coal powder panels, a over fire air (OFA) panel, a bottom air panel, and a warm up oil panel in 1 windbox. Figure 4.7 shows that the furnace geometry uses approximately 470,000 computational grid cells with 4 blocks. The highlighted area of the grid cell is the feed coal and air for combustion in the furnace, due to a high change of velocity and temperature. Then, the geometry and grid were generated, the case of problem is set up, the calculation is run until convergence. To ensure accurate simulation results, a grid independent solution is important way to check. The initial simulation with initial grid is run and ensured convergence (10^{-4} of residual error, steady of monitor points). Then the grid was refined and the results of outlet were compared. The grid solution value that is independent was chosen for further analysis.

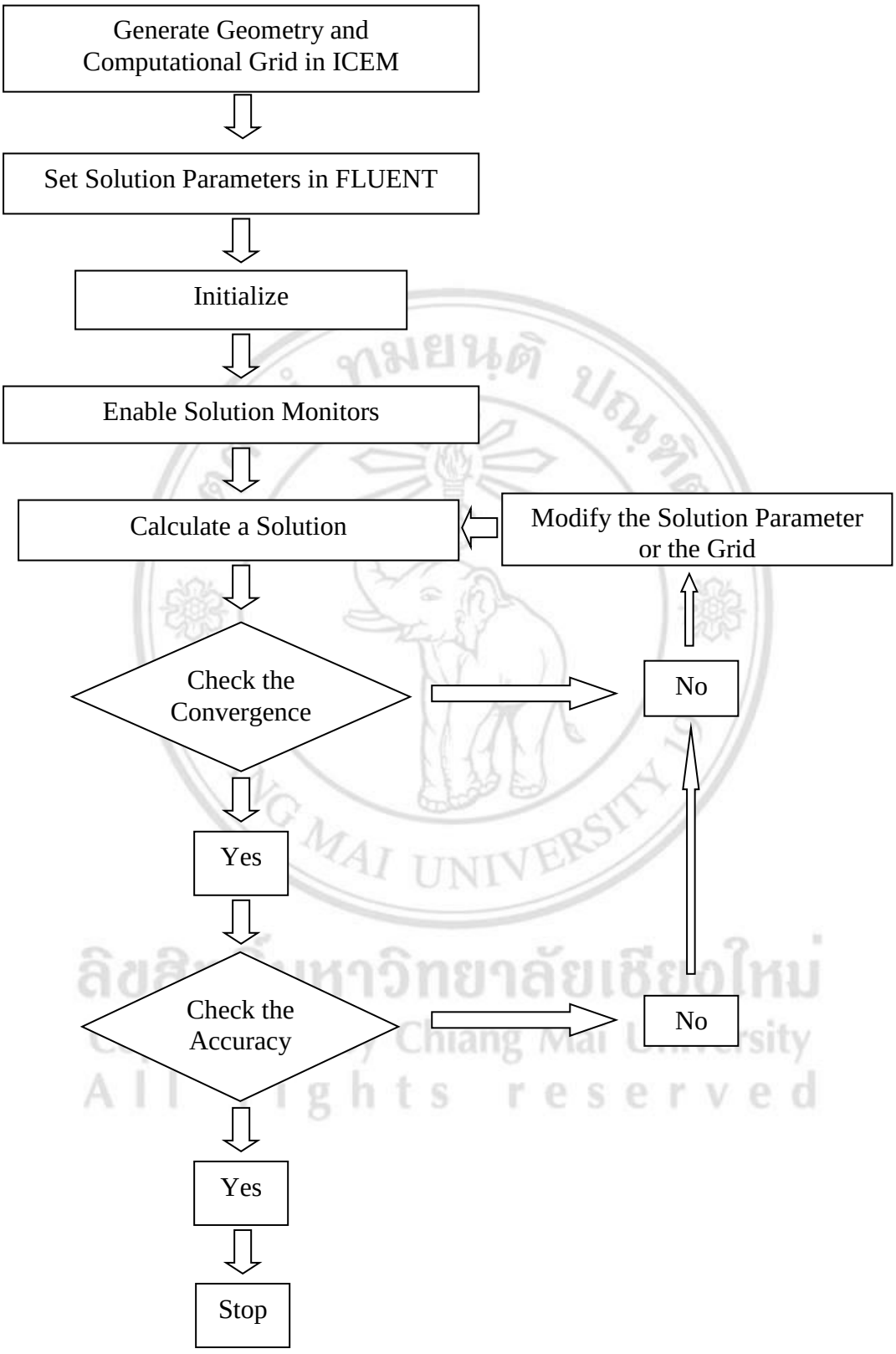

Figure 4.5 Flow chart of the CFD simulation

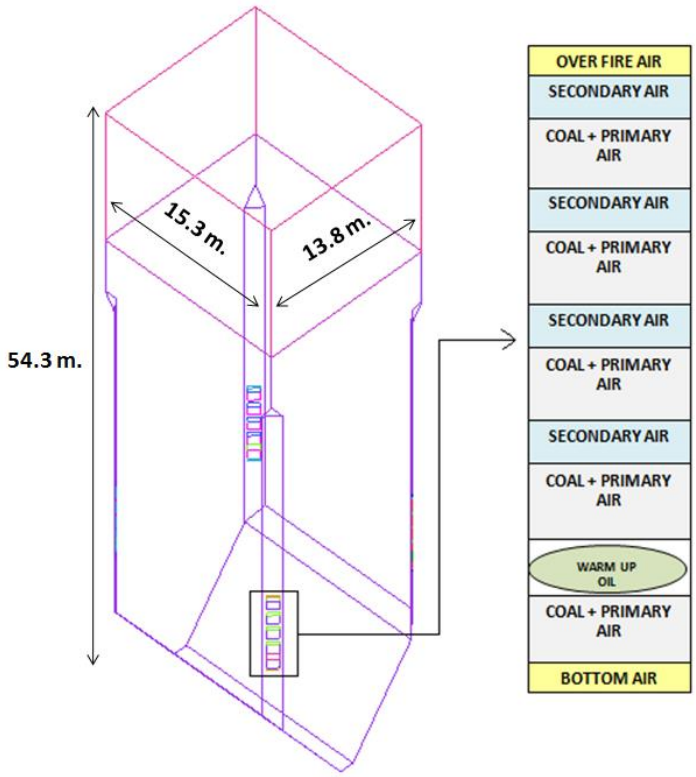

Figure 4.6 The Mae Moh boiler furnace was generated in ANSYS ICEM CFD program

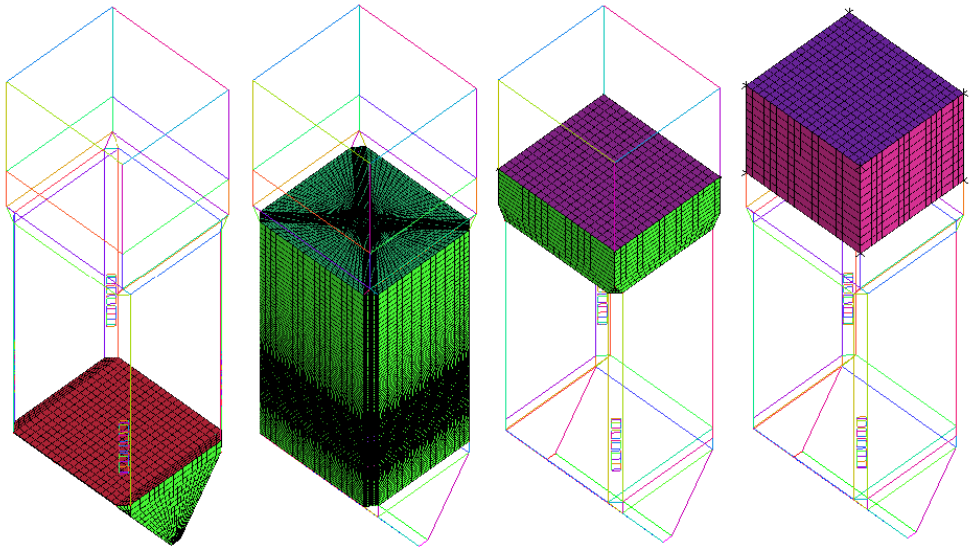

Figure 4.7 The grid cells were created in ANSYS ICEM CFD program

4.2.2 Operating and Boundary Conditions, and Sub-models

The grid of a boiler furnace is loaded from ICEM. Figure 4.7 shows the computational grid, inlet and outlet boundaries in FLUENT display. First case, the setting up of cold flow solution was simulated before turning on combustion. The model of standard k-ε turbulence and the energy equation were selected. From this case, the results were used in the grid independent study. Then, the combustion of Mae Moh lignite properties (disable radiation) was set up and solved. The simulation with turning on particle radiation was investigated in the next step.

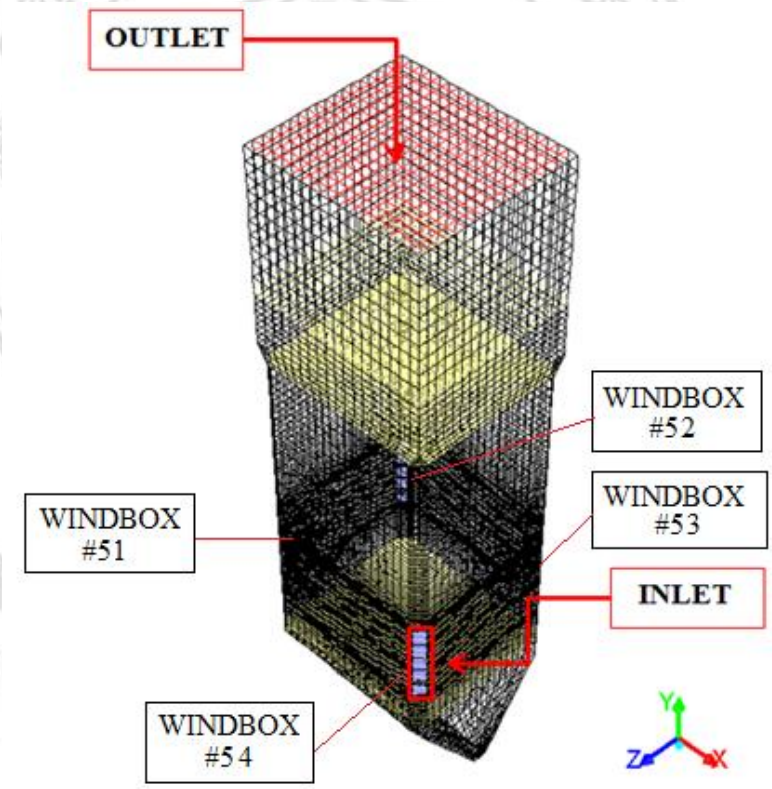

Figure 4.8 Defining inlet and outlet boundaries of boiler grid in FLUENT

The boundary conditions used for the CFD modeling are taken from the real operation at the Mae Moh power plant, shown in Tables 4.1 to 4.3. The inlet boundary condition was set to velocity inlet. The outlet boundary condition was set as the outflow calculation at the top of the geometry. The wall

boundary condition was divided into two parts. The bottom outlet was set as an escape wall, and all of the wall surfaces were set as the no-slip condition and having 4.572 mm. thickness. Temperature was 673 K, 0.8 of internal emissivity, and 1.5 W/m-K thermal conductivity of material. In this case study, the data about coal properties and operate parameter from EGAT was used. The coal particle was set with coal properties, as-received high calorific value, volatile molecular weight, CO/CO_2 split in reaction 1 products, high temperature volatile yield, fraction of N, Char, and dry density.

Table 4.1 Boundary conditions for the secondary air inlet

Parameter	Windbox corner 51	Windbox corner 52	Windbox corner 53	Windbox corner 54
Velocity specification method	components	components	components	components
Coodinate system	Cartesian	Cartesian	Cartesian	Cartesian
X (m/s)	49.56	41.12	-49.56	-41.12
Z (m/s)	-34.45	44.14	34.45	-44.14
Turbulence intensity	10%	10%	10%	10%
Hydraulic diameter (m)	1.92	1.92	1.92	1.92
Temperature (K)	576	576	576	576
O_2 Mass Fractions	0.2315	0.2315	0.2315	0.2315

Table 4.2 Boundary conditions for the coal + primary air inlet

Parameter	Windbox corner 51	Windbox corner 52	Windbox corner 53	Windbox corner 54
Velocity specification method	components	components	components	components
Coodinate system	Cartesian	Cartesian	Cartesian	Cartesian
X (m/s)	21.5	17.84	-21.5	-17.84
Z (m/s)	-14.94	19.15	14.94	-19.15
Turbulence intensity	10%	10%	10%	10%
Hydraulic diameter (m)	3.95	3.95	3.95	3.95
Temperature (K)	333	333	333	333
O_2 Mass Fractions	0.2315	0.2315	0.2315	0.2315

Table 4.3 Boundary conditions for the OFA

Parameter	Windbox corner 51	Windbox corner 52	Windbox corner 53	Windbox corner 54
Velocity specification method	components	components	components	components
Coodinate system	Cartesian	Cartesian	Cartesian	Cartesian
X (m/s)	49.56	41.12	-49.56	-41.12
Z (m/s)	-34.45	44.14	34.45	-44.14
Turbulence intensity	10%	10%	10%	10%
Hydraulic diameter (m)	0.6	0.6	0.6	0.6
Temperature (K)	576	576	576	576
O_2 Mass Fractions	0.2315	0.2315	0.2315	0.2315

The properties of the coal particles are presented in Table 4.4. The diameter of the particles was assumed to have the same size with a 200 mesh size. Due to the combustion reaction was chosen as 2 step reaction, so the combustion fraction was 36.7%, the burnout stoichiometric ratio was 1.33, the heat of reaction for burnout was 9.21 MJ/kg, and the reaction heat fraction absorbed by the solids for CO was 100%. After setting up all boundary conditions and properties of the materials, the solution was initialized and patched high temperature and product species mass fraction in reaction zone (near burners).

Table 4.4 Particle injection properties

Parameter	Windbox corner 51	Windbox corner 52	Windbox corner 53	Windbox corner 54
Injection Name	injection-0	injection-1	injection-2	injection-3
Particle Type	combusting	combusting	combusting	combusting
Material	coal-hv	coal-hv	coal-hv	coal-hv
Devolatilizing Species	CO	CO	CO	CO
Product Species	O_2	O_2	O_2	O_2
Point Properties				
- Temperature (K)	333	333	333	333
- X-velocity (m/s)	21.5	17.84	-21.5	-17.84
- Z-velocity (m/s)	-14.94	19.15	14.94	-19.15
Diameter (m)	$7.4e^{-5}$	$7.4e^{-5}$	$7.4e^{-5}$	$7.4e^{-5}$
Total Flow Rate (kg/s)	18.75	18.75	18.75	18.75

After the first case simulation, the superheater and reheater zones were set as porous media. The CFD simulations were simulated with real operational information (coal properties and real operation) to compare the results obtained with the measured heat flux and flue gas outlet. After that, the simulations were adapted for coal with low and high CaO (freeSO_3) in ash. The governing equations in CFD model (the mass, momentum, and energy conservation equation) were presented in Chapter 2. In order to predict flow, heat, and coal particle motion in the boiler furnace, the sub-models were used in this case.

1) The RNG k-ε model is employed in order to obtain accurate results because of the presence of swirling flows (Black et al, 2013; Garba, 2012; Degereji et al., 2012; Edge et al., 2012). From the Theory Guide (ANSYS, 2010), the RNG model provides an analytically derived differential formula for effective viscosity that accounts for low-Reynolds-number effects, and more accurate and reliable for a wider class of flows than the standard k-ε model. The Reynolds number is defined in Eq. (4.1) (Turns, 2006; Garba, 2012).

$$R_e = \frac{\rho u L}{\mu} \tag{4.1}$$

where ρ is the density, u is the velocity, L is the length scales, and μ is the viscosity.

The model is based on transport equations of turbulence kinetic energy (k) and its dissipation rate (ε). The model constant values in FLUENT are $C_{1\varepsilon}$ = 1.42, and $C_{2\varepsilon}$ = 1.68.

2) Discrete ordinates (DO) is one of the radiation model for solves the radiative transfer in the Cartesian system. The model was used to solve problems ranging form surface-to-surface radiation to participating radiation in combustion problems (ANSYS, 2010). The radiative transfer equation is shown in Eq. (4.2) (Chui et al., 1993; Garba, 2012).

$$\frac{dI(r,s)}{ds} = -(K_a + \sigma_s)(r,s) + K_a I_b(r) + \sigma_s \bar{I}(r,s) \tag{4.1}$$

where r as position function, s is the direction function, K_a is the absorption coefficient, σ_s is the scattering coefficient, I_b is the black

body coefficient, and $\bar{I}$ is the black body in scattering coefficient. WSGGM was used in absorption model (Garba, 2012).

3) Eddy Dissipation is a model in species transport and finite-rate chemistry as related to volumetric reactions. In FLUENT, the net rate of species production ($R_{i,r}$) is shown below.

$$R_{i,r} = v'_{i,r} M_{w,i} A \rho \frac{\varepsilon}{k} min_{RR} \left(\frac{Y_{RR}}{v'_{R,r} M_{w,RR}}\right) \quad (4.2)$$

$$R_{i,r} = v'_{i,r} M_{w,i} AB \rho \frac{\varepsilon}{k} \frac{\sum PY_P}{\sum_j^N v''_{j,r} M_{w,j}} \quad (4.3)$$

where v' is stoichiometric coefficient, i is species, r is reaction, M_w is the molecular weight, Y_{RR} is the mass fraction of a particular reactant, Y_P is the mass fraction of any product species, v'' is the stoichiometric for product j, A and B are empirical constant equal to 4 and 5 respectively.

The chemical equations for coal burned with O_2 in a 2 steps of chemical reaction are given in Eq. (4.4) to (4.5).

$$C + H + O + N + S + O_2 \rightarrow CO + 0.5H_2O + 0.5N_2 + SO_2 \quad (4.4)$$

$$2CO + O_2 \rightarrow 2CO_2 \quad (4.5)$$

4) The discrete phase model of Lagrangian in FLUENT, followed the Euler-Lagrange approach, is solved by tracking a large number of particles through the calculated flow field. The Eq. (4.6) shows the force balance equation (in x-direction) that included a force of gravity on the particle.

$$\frac{du_p}{dt} = F_D\left(u - u_p\right) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \tag{4.6}$$

where $F_D\left(u - u_p\right)$ is the drag force per unit mass of particle, u is the fluid phase velocity, u_p is the particle velocity, ρ is the density, g_x is the gravitational force, and F_x is an additional acceleration (force per unit particle mass) term.