

## SIMPLIFIED LOGISTICS MODEL AND ITS APPLICATION IN PROCESS SIMULATION

by

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*In order to solve the problem of complex calculation of logistics value in process simulation, based on the parameter characteristics of ASPEN PLUS, a simplified logistics calculation model is proposed. The comparison with exercom shows that the error of the calculation results in this paper is less than 1%, which verifies the correctness of the model. The calculation model of logistics flow provides convenience for process simulation software ASPEN PLUS to analyze the simulation process. Based on the logistics calculation model and the "fuel cost" model of thermal economics, a coal-fired boiler of a domestic unit is analyzed. The results show that the heat loss of the boiler mainly occurs in the process of coal decomposition and combustion, followed by the heat exchange process between flue gas and main heat exchange surface. The overall efficiency of the boiler is 46.4%.*

**Key words:** *logistics, exercom, boiler, human capital, industry resilience, industrial agglomeration*

### Introduction

With the development of economy, human beings get more and more energy from the nature, and the environment has been seriously damaged. With the global environment and energy situation of the tension, the use of energy conservation gradually caused people's attention. Exergic analysis can reflect the perfection of the energy system from a certain angle. In order to achieve exergy analysis of the energy system, exergy flow of various forms in the system should be calculated and analyzed. The process simulation software provides a simple scheme for modelling thermal system and chemical process, but generally the software cannot directly calculate the exergy flow in the thermal system. In order to achieve exergy analysis of the energy system in the process simulation software, domestic and foreign scholars have put forward numerous calculation schemes. Exergy circulation in the system can usually be divided into thermal exergy, exergy and logistics exergy. Exergy and heat exergy are relatively simple to calculate [1]. Logistic exergy is better known as the computational model proposed by Kotas and Hinderink, [see ref. 2]. Kotas divides logistics exergy into physical exergy and chemical exergy, and the basic calculation process is shown in fig. 1. For the convenience of analysis, the chemical exergy defined by Kotas is divided into two parts [3]. Hinderink *et al.* [4, 5] divided logistics exergy into physical exergy, chemical exergy and hybrid exergy, and compiled

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commercial software ExerCom using this model. Palacios-Berechez [6] summarized various logistic exergy calculation schemes and compared the exergy calculation results of various methods. Sen [7] used FactSage to calculate logistics exergy using the same method as Kotas. The way Querol calculates exergy values is basically the same as Kotas, but Querol believes that a hybrid exergy is already included within a physical exergy. Abdollahi-Demneh [8] also adopted the idea of Kotas in calculation of logistics exergy, but he divided the chemical exergy into four parts in calculation. Abdollahi-Demneh [8] wrote an external computing program for HYSYS to calculate logistics exergy. Montelongo-Luna [9] used Hinderink's method to prepare exergy analysis calculation program for the open source process simulation software Sim42, but he chose a different benchmark environment from Hinderink in his calculation. Wang *et al.* [2] in China used Hinderink's method to add exergic calculation function HYSYS process simulation software by VB programming, and analyzed the methane process using this method. Ghannadzadeh *et al.* [10] summarized the previous methods for calculating logistics exergy in process simulation software, proposed a new scheme for computing logistics exergy, and compiled the calculation program for process simulation software ProSimPlus. The basic idea of the method is also from Kotas's calculation model. As shown in figs. 1 and 2, whether Kotas model or Hinderink model, the calculation of logistics exergy is very complicated. Generally, we do not need to know the specific composition of physical exergy, chemical exergy and hybrid exergy when solving logistics exergy. In order to facilitate and efficiently implement exergy analysis, it is necessary to simplify the calculation process of logistics exergy. This paper puts forward a new model to calculate logistics exergy, and makes the calculation process of logistics exergy simple through analysis and simplification.

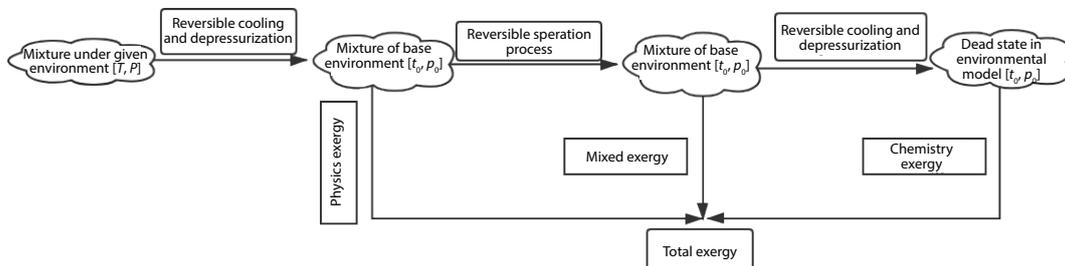


Figure 1. Solving process of Kotas calculation model

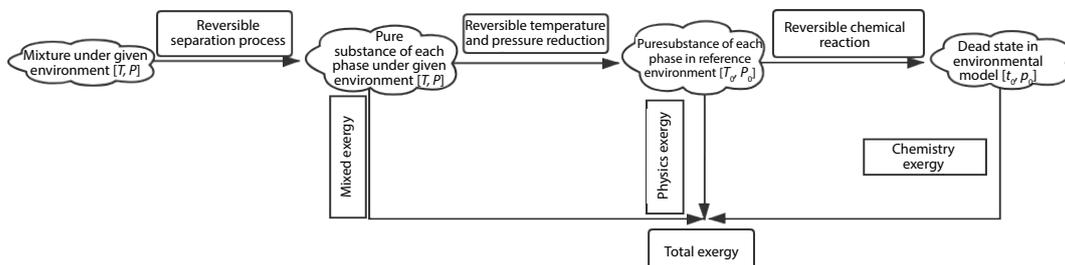


Figure 2. The process to calculate the exergy of a material stream with Hinderink's model

### Thermodynamic calculation model and its application

Logistics exergy can be divided into internal exergy and external exergy [11], while external exergy refers to kinetic energy exergy and potential exergy, which are always ignored

in calculation. Therefore, the commonly used logistics exergy refers to its internal exergy. As shown in fig. 3. The calculation model in this paper divides logistics exergy into three parts, namely chemical exergy, physical exergy and hybrid exergy, which, respectively represent the ideal work of the three reversible processes. It should be noted that the solution process in this paper is slightly different from Hinderink's calculation method, because the separation process in this paper does not consider the phase balance between each pure substance. Even if a pure substance has phase balance in its environment, it will reach the same phase state through certain changes during the separation process.

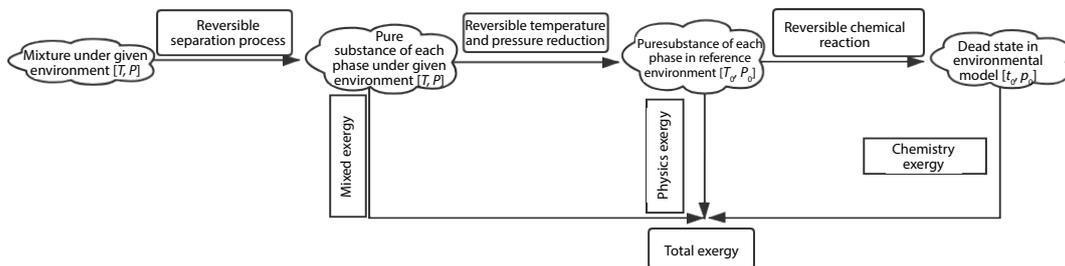


Figure 3. The process to calculate the exergy of a material stream with this paper's model

### Chemical exergy model

Exergy of pure substance is defined as the ideal work needed for a substance and environment to reach the non-binding equilibrium through chemical reaction and/or physical diffusion [12]. The Szargut model or the Tanyama-Yoshida model is used to evaluate the chemical exergy of pure material  $A_i$  [1, 3]:

$$Ex_{ch}(A_i) = Ex_0(A_i) + \Delta G_0(A_i) \quad (1)$$

In model (1):

$$Ex_0(A_i) = \sum_{el} v_{el} Ex_{el}$$

where  $Ex_0(A_i)$  is the variable associated with the composition of the chemical elements of the pure substance,  $v_{el}$  – the number of elements in a substance,  $Ex_{el}$  [kJmol<sup>-1</sup>] – the exergy of the element contained in the substance, and  $A_i$  – the material component  $i$  in logistics.

The calculation of each element chemical exergy in  $Ex_0(A_i)$  can be found from the exergy value table of the element. Szargut system can be referred to [1], and Kaguyama-Yoshida system can be referred to [3]. As the standard gibbs free energy used by these systems in calculating the chemical exergy of elements does not come from the set value inside ASPEN PLUS, certain error may occur when looking up the table directly, but the error is very small, so direct use is feasible. In order to improve the accuracy, the exergy of each element can be recalculated according to the internal data of ASPEN PLUS [1], which is adopted in this paper. Table 1 compares the data in reference [1] with the calculations using ASPEN PLUS internal data.

Table 1. The comparison between published values and values calculated based on ASPEN PLUS

Element type	[13]	The calculation results
C/kJ·mol <sup>-1</sup>	410.260	410.292
H/kJ·mol <sup>-1</sup>	118.095	118.103
O/kJ·mol <sup>-1</sup>	1.985	1.987
N/kJ·mol <sup>-1</sup>	0.360	0.360

The chemical exergy of complex logistics is the sum of all pure logistics in complex logistics before mixing [3]. For a flow rate of  $F$  containing components  $A_1, A_2... A_n$ , the molar fractions of each component are  $X_1, X_2... X_n$ . Exergy of  $X_N$ 's logistics  $M$  can be calculated:

$$Ex_{\text{ch}} = F \sum_{i=1}^n x_i Ex_{\text{ch}}(A_i) = F \sum_{i=1}^n [x_i Ex_0(A_i) + x_i \Delta G_0(A_i)] \quad (2)$$

where  $Ex_{\text{ch}}(\cdot)$  [kJmol<sup>-1</sup>] is the chemical exergy of the substance,  $\Delta G_0(\cdot)$  [kJmol<sup>-1</sup>] – the Gibbs free energy of matter,  $x_i$  – the mole fraction of components in logistics, and  $F$  [mols<sup>-1</sup>] – the logistics flow.

### Physical exergy model

Physical exergy in complex logistics refers to the sum of all pure physical exergies in the logistics before mixing [3]. Physical exergy in pure material is defined as the ideal work required in the process of a substance from the reversible temperature and pressure of the reference environment ( $T_0, p_0$ ) to the specified system state ( $T, p$ ). For pure material  $A_i$ :

$$Ex_{\text{ph}}(A_i) = (h_i - h_{i0}) - T_0(s_i - s_{i0}) = (h_i - T_0s_i) - (h_{i0} - T_0s_{i0}) = (h_i - T_0s_i) - g_{i0} \quad (3)$$

where  $Ex_{\text{ph}}(\cdot)$  [kJmol<sup>-1</sup>] is the physical exergy of the substance,  $h_i$  [kJmol<sup>-1</sup>] – the enthalpy of substance  $i$  in a given environment,  $s_i$  [(kJmol<sup>-1</sup>)K<sup>-1</sup>] – the entropy of substance  $i$  in a given environment,  $h_{i0}$  [kJmol<sup>-1</sup>] – the enthalpy of substance  $i$  under standard conditions,  $s_{i0}$  [(kJmol<sup>-1</sup>)K<sup>-1</sup>] – the entropy of substance  $i$  in the standard environment, and  $g_{i0}$  [kJmol<sup>-1</sup>] – the Gibbs free energy for substance  $i$  under standard conditions.

Here, if it is stipulated that the Gibbs free energy of a substance in standard state ( $T_0, P_0$ ) is the Gibbs free energy generated by its standard, namely:

$$\Delta G_0(A_i) = g_{i0} \quad (4)$$

Then eq. (3) can be simplified to model (5):

$$Ex_{\text{ph}}(A_i) = [h_i - T_0s_i] - \Delta G_0(A_i) \quad (5)$$

Aforementioned rules in ASPEN PLUS is established, the help files in the ASPEN PLUS point under the ( $T_0, p_0$ ) of the individual elements of a substance to ideal gas state exists, enthalpy and gibbs free energy of the zero, each material under the environment of standard enthalpy and gibbs free energy values through standard formation enthalpy and gibbs free energy generated. Then, as for logistics  $M$ , its physical exergy can be expressed:

$$Ex_{\text{ph}} = F \sum_{i=1}^n x_i Ex_{\text{ph}}(A_i) = F \sum_{i=1}^n [x_i (h_i - T_0s_i) - x_i \Delta G_0(A_i)] \quad (6)$$

### Mixed exergy model

There are irreversible losses due to mixing and chemical reactions in the mixing process of substances. Exergy mixing is the ideal work needed for each pure logistics in the studied logistics to mix with each other and reach phase balance under the specified environment [3]. Exergy expression of logistics  $M$  is as follows if the average enthalpy value and the average entropy value of post-mixing logistics are  $H$  and  $S$ :

$$Ex_{\text{mi}} = F \left[ \left( h - \sum_{i=1}^n x_i h_i \right) - T_0 \left( s - \sum_{i=1}^n x_i s_i \right) \right] = F \left[ (h - T_0s) - \sum_{i=1}^n x_i (h_i - T_0s_i) \right] \quad (7)$$

where  $Ex_{\text{mi}}$  [kJmol<sup>-1</sup>] is the mixing exergy of the substance,  $h$  [kJmol<sup>-1</sup>] – the average enthalpy of logistics in a given environment, and  $s$  [kJ(molK<sup>-1</sup>)<sup>-1</sup>] – the average entropy value of logistics in a given environment.

In ASPEN PLUS,  $h - T_0s = \text{AVAILMX}$  is defined as an available energy function, and the eq. (7) can be represented:

$$Ex_{mi} = F \left[ \text{AVAILMX} - \sum_{i=1}^n x_i (h_i - T_0 s_i) \right] \quad (8)$$

### Logistic exergy simplified model

In this paper, the calculation model of chemical exergy, physical exergy and hybrid exergy in logistics is established through three reversible processes, respectively, and the exergy in these three parts is the exergy in logistics:

$$Ex_F = Ex_{ch} + Ex_{ph} + Ex_{mi} \quad (9)$$

where  $Ex_F$  [ $\text{kJmol}^{-1}$ ] is the exergy value of logistics. By putting eqs. (2), (6), and (8) into eqs. (9) and (10) can be obtained:

$$Ex_F = F \sum_{i=1}^n [x_i Ex_0(A_i) + x_i \Delta G_0(A_i)] + F \sum_{i=1}^n [x_i (h_i - T_0 s_i) - x_i \Delta G_0(A_i)] + F \left[ \text{AVAILMX} - \sum_{i=1}^n x_i (h_i - T_0 s_i) \right] \quad (10)$$

By simplifying eqs. (10) and (11) can be obtained:

$$Ex_F = F \left[ \sum_{i=1}^n x_i Ex_0(A_i) + \text{AVAILMX} \right] \quad (11)$$

Equation (11) shows that after the environment model is selected, the exergy factors affecting a logistics have two main parts: the first part is the end parameter AVAILMX and the other part is its chemical composition. Of course, the selected thermodynamic method also has a certain influence on the results [1]. The previous equation also verifies that logistic exergy is a state parameter that has no relationship with all the reversible processes that are gone through when obtaining the logistic exergy. Therefore, whether the calculation model adopted by Kotas, Hinderink *et al.* [4, 5], or the model in this paper, as long as the selected environment model and the thermodynamic calculation method are the same, the overall logistics exergy value for the same physical system should be the same.

### Validation of model

To verify the correctness of the model, several calculation examples of commercial software ExerCom [14] were investigated and compared with the results obtained through the ExerCom method presented in this paper. Some basic parameters of these calculation examples are shown in tab. 2. Table 3 lists the comparison results of the calculation model and ExerCom in this paper.

The previous calculation results show that the calculation result based on the model in this paper differs less than 1% from that of commercial software ExerCom, which verifies the correctness of the model built in this paper. This proves that the logistics exergy calculation model established in this paper is feasible for exergy analysis of ASPEN PLUS process simulation results.

**Table 2. The basic parameters of some material streams**

Group number	Temperature [°C]	Pressure [kPa]	Traffic [ $\text{mols}^{-1}$ ]	H <sub>2</sub> O [ $\text{mols}^{-1}$ ]	CO <sub>2</sub> [ $\text{mols}^{-1}$ ]	C <sub>6</sub> H <sub>14</sub> [ $\text{mols}^{-1}$ ]
1	250	500	13.475	12.1272	1.34747	–
2	100	300	0.3223	–	–	0.32
3	50	100	1.9041	0.234271	1.34747	0.32
4	50	100	11.893	11.8929	–	–

**Table 3. The comparison of the results**

Group number	AVAILMX [kJmol <sup>-1</sup> ]	Literature value [kW]	Value [kW]	Relative error [%]
1	-239.984	211.726	211.753	-0.013
2	-1.910	1326.930	1325.562	0.103
3	-309.195	1352.780	1351.408	0.101
4	-237.104	11.591	11.653	-0.534

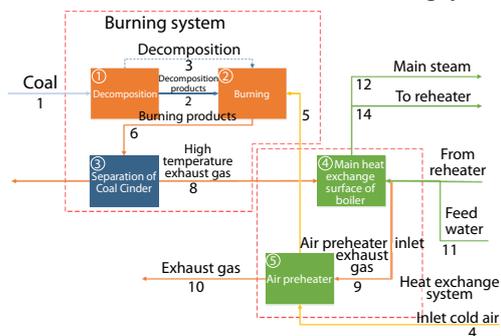
### Example analysis

The boiler is the largest part of the coal-fired power plant. Through the simulation of the boiler, the specific position of the internal damage of the boiler can be determined, which provides the basis for improving the combustion technology of the boiler. In China, there are few reports on this aspect. In [15], the damage of combustion process is analyzed by numerical method, and the main factors affecting the flame loss in combustion process are analyzed. In foreign countries, [16] analyzed the process of combustion loss and entropy increase by establishing a mathematical model, and analyzed the combustion process in detail.

Based on the aforementioned logistics calculation model, a simple coal-fired boiler is analyzed, and the value of each logistics in the boiler model is calculated. Based on the *fuel product* model of thermoeconomics, this paper analyzes each subsystem and points out the main part of the boiler loss.

### Simplified boiler model

As shown in fig. 4, a simplified model of coal-fired boiler is established in ASPEN PLUS. The boiler model can be simply summarized as the process of high temperature flue gas generated by combustion of fuel in furnace, and heat exchange between flue gas and heat exchanger [17]. Therefore, the coal-fired boiler system can be roughly divided into combustion system and heat exchange system. As shown in the figure, the unit operation model RGIBBS is used to simulate the coal combustion process, and the RGS module uses the homogeneous Gibbs free energy minimum to calculate the equilibrium.



**Figure 4. The flow chart of a simplified model of a boiler**

In fig. 4, the combustion system is divided into three sub processes. Firstly, the coal is decomposed into some conventional logistics mixture by RYFIELD module. The reaction heat generated during decomposition is connected with RGIBBS module through heat flow to ensure the heat balance of the system. SSPLIT diverter is used to simulate the boiler slag discharge process. After separation, ash is discharged from the system and flue gas enters the following process.

The boiler heat exchange system is simply divided into two sub processes, one is that the flue gas heats the feed water and reheated steam through the main heat exchange surface (mheatx) of the boiler, and the other is that the flue gas preheats the cold air through the air preheater (heatx). In the model, the oxygen content in the flue gas is set as 5%, and the excess air coefficient is 1.313. Some main design parameters of the boiler are shown in tab. 4.

**Table 4. The main design parameters of the boiler**

Project	Value under design condition
Superheated steam flow [th <sup>-1</sup> ]	1700.5
Outlet pressure of superheated steam [MPa]	24.2
Superheated steam outlet temperature [°C]	566
Reheat steam flow [th <sup>-1</sup> ]	1399.754
Reheat steam inlet pressure [MPa]	4.434
Reheat steam outlet pressure [Mpa]	3.99
Reheat steam inlet temperature [°C]	315.9
Reheat steam outlet temperature [°C]	566
Feed water temperature [°C]	282.4
Outlet flue gas temperature of air preheater [°C]	130.0

Fuxin bituminous coal is used in the boiler combustion process. The industrial analysis mass fraction of this coal is shown in tab. 5. The unconventional components can be used to treat coal and cinder in ASPEN PLUS. The high calorific value of coal is estimated [18]:

$$Q_{GW} = 0.3491w(C) + 1.1783w(H) + 0.1005w(S) - 0.1034w(O) - 0.0151w(N) - 0.0211w(A) \quad (12)$$

**Table 5. The elemental analysis and industry analysis of the coal**

Mass fraction of industrial analysis [%]					
C <sub>d</sub>	H <sub>d</sub>	O <sub>d</sub>	N <sub>d</sub>	S <sub>d</sub>	A <sub>d</sub>
48.300	3.300	8.600	0.800	1.000	23.000

### Boiler model analysis

It can be seen from fig. 4 that 14 logistics and five subsystems are involved in the previous boiler model. In order to facilitate the analysis of the model, all logistics and subsystems are numbered in the figure. As the coal and ash are unconventional components, the value cannot be obtained by the aforementioned methods. Since the energy of slag discharge and exhaust gas is almost impossible to be reused, in order to simplify the analysis, it is set that the values of slag discharge and exhaust gas are both 0, and the value of coal is estimated [17]:

$$Ex = 363.439w(C) + 1075.633w(H) - 86.308w(O) + 4.147w(N) + 190.798w(S) - 21.1w(A) \quad (13)$$

According to the aforementioned settings, the simulation model of boiler combustion and heat transfer process is established by ASPEN PLUS, and the simulation results are shown in tab. 6.

From the previous simulation results, it can be seen that the simulation results of coal consumption and smoke exhaust rate of the boiler are 213.63 tonne per hour and 2329.64 tonne per hour, respectively. In the actual operation, the coal consumption of the boiler is 220 tonne per hour, and the smoke exhaust volume is 2400 tonne per hour. The error between the simulation results and the actual value is less than 3%. In addition, for the temperature of flue gas after adiabatic combustion, the simulation result is 1974.9 °C, which is basically consistent with the analysis result in [18]. In conclusion, the accuracy of the model meets the needs of this analysis.

**Table 6. The exergy of each flow in the system**

Stream name	Mass-flow [t <sup>h</sup> <sup>-1</sup> ]	Exergy [GJh <sup>-1</sup> ]
Coal	213.63	4287.62
Decomposition products	213.63	6260.83
Inlet cold air	2132.67	7.85
Hot air	2132.67	173.33
Flue gas coal slag mixture	2346.31	3162.47
DESLAGGING	16.66	0.00
High temperature flue gas	2329.64	3162.47
Flue gas at air preheater inlet	2329.64	412.33
Smoke extraction	2329.64	0
Boiler feed water	1700.50	567.58
Main steam	1700.50	2184.73
Reheat steam cold section	1399.71	1288.78
Hot section of reheat steam	1399.71	1662.74

Based on the aforementioned simulation results, the exergy loss, exergy loss rate and exergy efficiency of the main parts of the system are analyzed according to the *fuel product* model in thermoconomics. The results are shown in tab. 7.

**Table 7. The exergy analysis result of each subsystem in the boiler system**

Number	Subsystem	Fuel [kJh <sup>-1</sup> ]	Product [kJh <sup>-1</sup> ]	Damage [kJh <sup>-1</sup> ]	Efficiency	Loss rate
1, 2, 3	Combustion system	4460.95	3162.47	1298.48	0.709	0.302
4	Main heat exchange surface of boiler	2750.14	1991.11	759.03	0.724	0.177
5	Air preheater	232.64	165.48	67.16	0.711	0.016
	Smoke exhaust process	179.69	0.00	179.69	0.000	0.042
	Whole	4295.47	1991.11	2304.36	0.464	0.536

From the calculation results in the previous table, it can be seen that the largest part of the boiler model is coal decomposition and combustion process, and the loss rate is 30.2%. This is consistent with the results of [15, 16]. The magnitude of loss in combustion process can account for 20-30% of the total input system. The second is the heat transfer process between flue gas and main heat exchange surface, and the loss rate is 17.7%. In addition, through the analysis of the boiler as a whole, the overall efficiency of the boiler is 46.4%.

## Conclusions

The logistics calculation model is established, and the correctness of the model is verified by comparing with the calculation results of exercom. Based on this model, a boiler combustion model is analyzed. The main results and conclusions are as follows.

- According to the characteristics of parameter calculation in chemical process simulation software, the calculation and analysis of logistics in ASPEN PLUS are simplified.
- This model is used to analyze a boiler combustion model. It is concluded that the most serious damage part in the boiler model is the decomposition and combustion process of coal. The loss rate is 30.2%, followed by the heat exchange process between flue gas and main heat exchange surface. The loss rate is 17.7%, and the overall boiler efficiency is 46.4%.

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