Numerical Modelling of Combustion in a Zinc Flash Smelter

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ABSTRACT

The development of a mathematical model for the flash smelting of zinc concentrate is described. Computational fluid dynamics has been used to solve the two-phase flow and combustion equations. Special codings for zinc concentrate smelting and combustion of natural fuel gas have been developed. In the simulation, the fuel gas is combusted using the eddy-breakup model and the gas-particle reactions are limited by a combination of heat transfer and mass diffusion. For the zinc concentrate combustion submodel, the concept of a composite particle was adopted to include the contributions from all minerals present in the concentrate. It is assumed that after heating to a temperature of 530°C, the pyrite in the composite particle decomposes and ignites. When the particles are further heated to a temperature of 1600°C, they melt and zinc sulphide vaporizes to form gaseous sulphur and zinc. The sulphur combusts to form sulphur dioxide and heat is released to the gas phase. The rate of vaporization is limited by the supply of heat to the particle. After all the zinc has left the particle, the oxidation of FeS in the concentrate commences and is controlled by the rate of oxygen diffusion to the particle surface. Modelling results of the combustion within the environment of a gas-fired furnace are presented as an example of the simulations performed for flash smelting of zinc concentrate.

1. INTRODUCTION

Flash smelting of zinc concentrate to produce zinc or zinc oxide is an alternative treatment to the electrolytic route. In the flash furnace, oxygen, natural gas and zinc concentrate are injected through a burner at the top of the reaction shaft. Natural gas is burned to provide heat for the particle reactions. Intense reactions occur while the particles are in suspension producing zinc vapour and other gases. Good dispersion of the particles is an essential factor in promoting ignition of the concentrate in the upper part of the shaft.

A numerical model has been developed using the computational fluid dynamics code CFX 4.1 (AEA Technology, 1995) to solve the two-phase flow and combustion equations. Special codings for zinc concentrate smelting and a combustion model for natural fuel gas have been generated so that the models can be used together. The equations for the gas and particle reactions are solved simultaneously and the combined model has been used to investigate the smelting characteristics in a zinc smelter. Various parameters including particle size and oxygen concentration in the injected gas have been investigated. The combined model may now be used to optimise smelting performance, evaluate burner designs, carry out parametric studies and trouble-shooting exercises.

2. CONCENTRATE COMPOSITION

The model was based upon the combustion of a typical Broken Hill zinc concentrate, the chemical composition of which is shown in Table 1. This material usually has an average size of about 50 μm.

Table 1. Chemical analyses of zinc concentrate (wt.%)

Zn	Pb	Fe	Cu	Cd	S
49.4	1.6	11.3	0.26	0.16	33.3

CaO	SiO_2	Al_2O_3	Mn	MgO
0.2	1.53	0.3	0.7	0.08

For ease of computation the concentrate was assumed to have the following simplified mineralogical composition - sphalerite (ZnS), 74.8 %; pyrite (FeS_2), 8.3 %; pyrrhotite (FeS), 14.0 %; the remaining 2.9 % being gangue.

3. NUMERICAL MODELLING METHOD

3.1 Gas and Particle Transport

The conservation equations for mass, momentum, enthalpy and turbulence quantities were solved using the Eulerian approach for the gas flow and the Lagrangian approach for the solid particles. These equations were solved numerically using the particle-source-in-cell technique (Crowe *et al*, 1977). The heat and mass sources from the gas combustion and zinc concentrate combustion were incorporated in an overall steady-state flow model. The turbulent gas flow was treated using the standard k-ε turbulence model.

3.2 Zinc Concentrate Combustion

Zinc concentrate combustion occurs in conjunction with the fuel gas combustion in the furnace. For the gas-particle reactions, a particle tracking approach was used to follow the temperature and the extent of reaction of the particles.

Table 2. Flash smelting reactions.

1. Initial heating - no reaction:
2. Pyrite decomposition at 530°C: $FeS_2 \rightarrow FeS + 0.5\ S_2$
3. Burning of pyritic sulphur: $0.5\ S_2 + O_2 \rightarrow SO_2$
4. Sphalerite-wurtzite transformation at 900°C: $ZnS_{(Sphalerite)} \rightarrow ZnS_{(Wurtzite)}$
5. Melting and vaporization at 1600°C: $ZnS(s) \rightarrow Zn(g) + 0.5\ S_2(g)$
6. Burning of sulphur from zinc sulphide: $0.5\ S_2 + O_2 \rightarrow SO_2$
7. Reaction of FeS: $FeS + {}^3/_2\, O_2 \rightarrow FeO + SO_2$

Since CFX 4.1 can only consider one type of particle, the concept of a composite particle was adopted for including the contributions from all the minerals present in the concentrate. This approach is similar to that taken in modelling the flash smelting of nickel concentrate by Koh and Jorgensen (1994).

In the model, the chemical reactions occurring in the composite particle were represented by a number of stages and some assumptions were necessary to simplify the model. The flash smelting reactions in the shaft are given in Table 2 and a diagram of the stages involved is shown in Figure 1. Figure 2 shows the particle histories, that is, the variation of particle parameters as they pass through the furnace. The parameters shown are particle temperature and the mass fractions of sulphur and zinc removed during combustion.

Initially, the particles heat up by convection and radiation to a temperature of 530°C without reaction. The pyrite decomposes and ignites at this temperature (Jorgensen and Moyle, 1982). The labile sulphur from the pyrite decomposition combusts with oxygen some distance from the particle releasing heat to the gas phase. Some of the heat is transferred back to the particles by convection and radiation from the gas.

The decomposition reaction is endothermic and the temperature of the particle remains at 530°C until all the pyrite has decomposed. To avoid modelling a separate reaction for sulphur combustion in the gas phase, this reaction (reaction 3) was added to the decomposition reaction (reaction 2) in the model. Thus, the overall reaction of pyrite to form sulphur dioxide was simulated in the model as follows:

$$FeS_2 + O_2 \rightarrow FeS + SO_2 \quad (1)$$

As a further simplification, the heat involved in the solid phase transition from sphalerite to wurtzite (which takes place at 900°C) has been assumed to occur at 530°C and the heat added to that required to decompose pyrite. This eliminates one decomposition reaction but slightly decreases the particle's ability to liberate labile sulphur by increasing the heat required. As the quantity of heat involved is small, this simplification has only a small effect in the model.

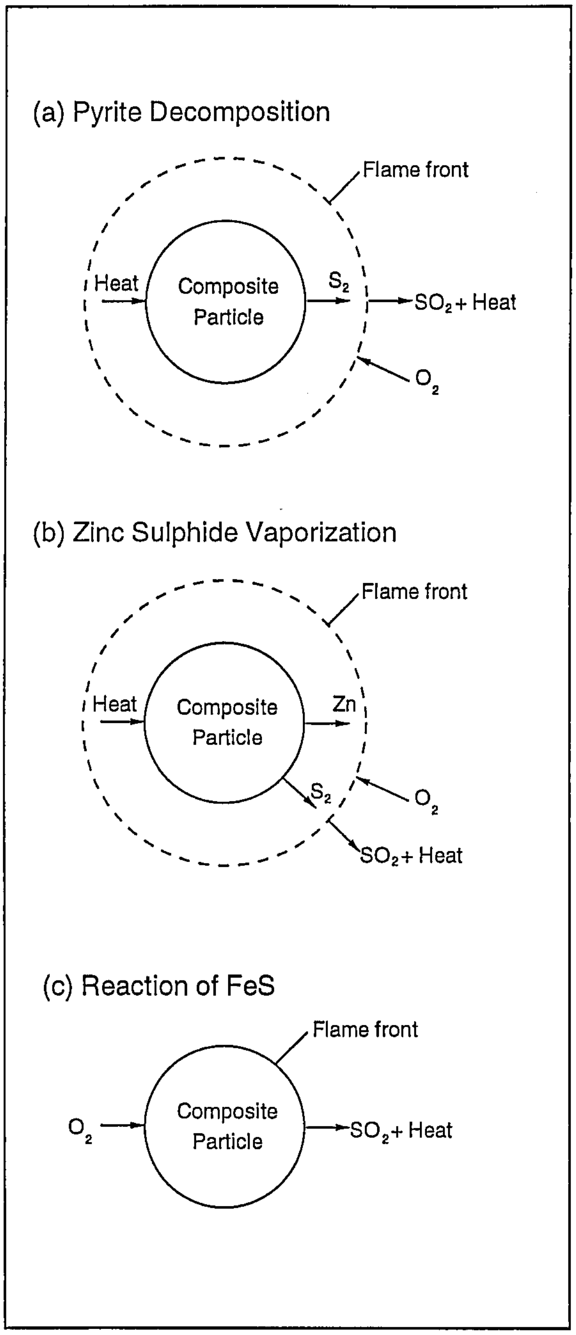

Figure 1. Stages in the combustion of a composite particle of zinc concentrate.

In the next stage of reaction, the particles are further heated to a temperature of 1600°C. At this temperature, the particles melt and zinc sulphide vaporizes to form gaseous sulphur and zinc. The sulphur in the gas phase combusts to form sulphur dioxide and the heat was released to the gas phase. Just as the pyrite decomposition-combustion reactions were simulated in the model by an overall reaction, so too were the vaporization-combustion reactions for zinc sulphide by an overall reaction, obtained by combining reactions 5 and 6 in Table 2 as follows:

$$ZnS + O_2 \rightarrow Zn(g) + SO_2 \qquad (2)$$

The temperature of the droplets remains at 1600°C until all the zinc has vaporized. The reaction is endothermic and the rate is limited by the supply of heat to the droplets.

In the final stage, the oxidation of FeS occurs and is controlled by the rate of oxygen diffusion to the droplet surface. This reaction is exothermic producing FeO in the droplet and sulphur dioxide in the gas phase and the heat is released to the droplet.

During all these reactions, the particle-droplet mass and diameter are continuously changing. The density of the particle has been assumed to be constant. In the coding of the concentrate submodel, all the sources and sinks in the exchanges between the particles and gas phase are accounted for.

3.3 Gas Combustion

Natural gas is mostly methane, the stoichiometric combustion of which occurs according to:

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2 \qquad (3)$$

The products of the stoichiometric combustion consist of 66.04% H_2O and 33.96% CO_2 by volume. The gas combustion submodel has been developed so that the gas and particle reactions can occur simultaneously. The gas reaction rate is determined by the chemical kinetics in conjunction with the eddy break-up model. Only the forward reaction indicated above is modelled and the rate constant is obtained from an Arrhenius expression:

$$k = A\,T^{B}\,e^{-E/RT} \qquad (4)$$

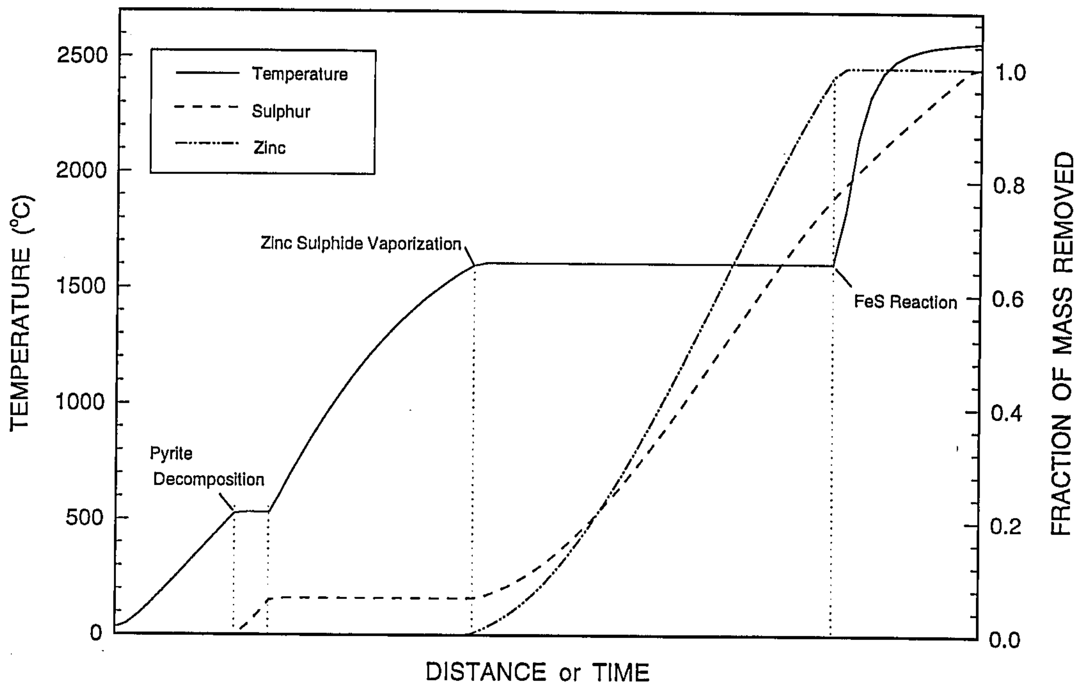

Figure 2. Schematic representation of the composite particle during combustion in terms of particle temperature and mass fractions of sulphur and zinc removed from the particle plotted against distance travelled by the particle or time lapsed.

In the eddy break-up model, the turbulent mixing time and the chemical induction time control the ignition and extinction of gas combustion (Bakke and Hjertager, 1987). All the heat from the reaction is released into the furnace where heat is transferred by convection and radiation to the surroundings. Further refinement of the combined combustion model is possible, although numerical convergence becomes more difficult with increased complexity.

4. RESULTS AND DISCUSSION

Combustion was simulated for a low-swirl burner with axial concentrate injection firing into a water-cooled shaft. Results were obtained for the gas and particle temperatures in the shaft, the amount of zinc vapour produced and the trajectories of the concentrate particles. The gas flow in Figure 3 is symmetrical about the centre line of the shaft, whereas the particles are allowed to move around in the 3-dimensional shaft.

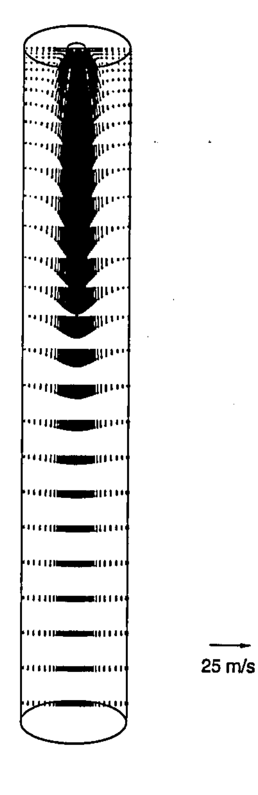

Figure 3. Velocity vectors of gas in the shaft.

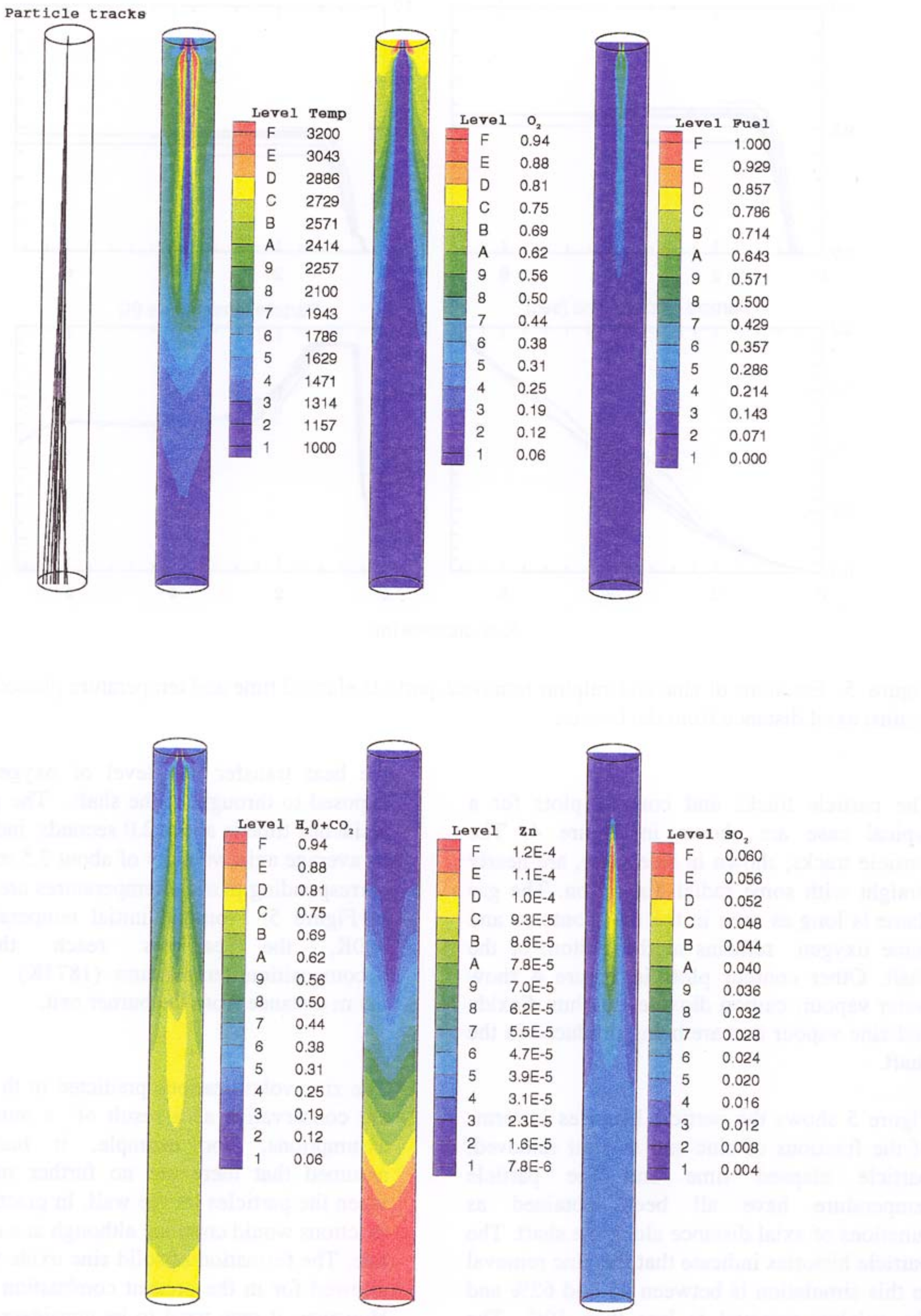

Figure 4. Particle tracks, gas temperature (K) distribution and volume fractions of oxygen, fuel, water vapour, carbon dioxide, zinc vapour and sulphur dioxide.

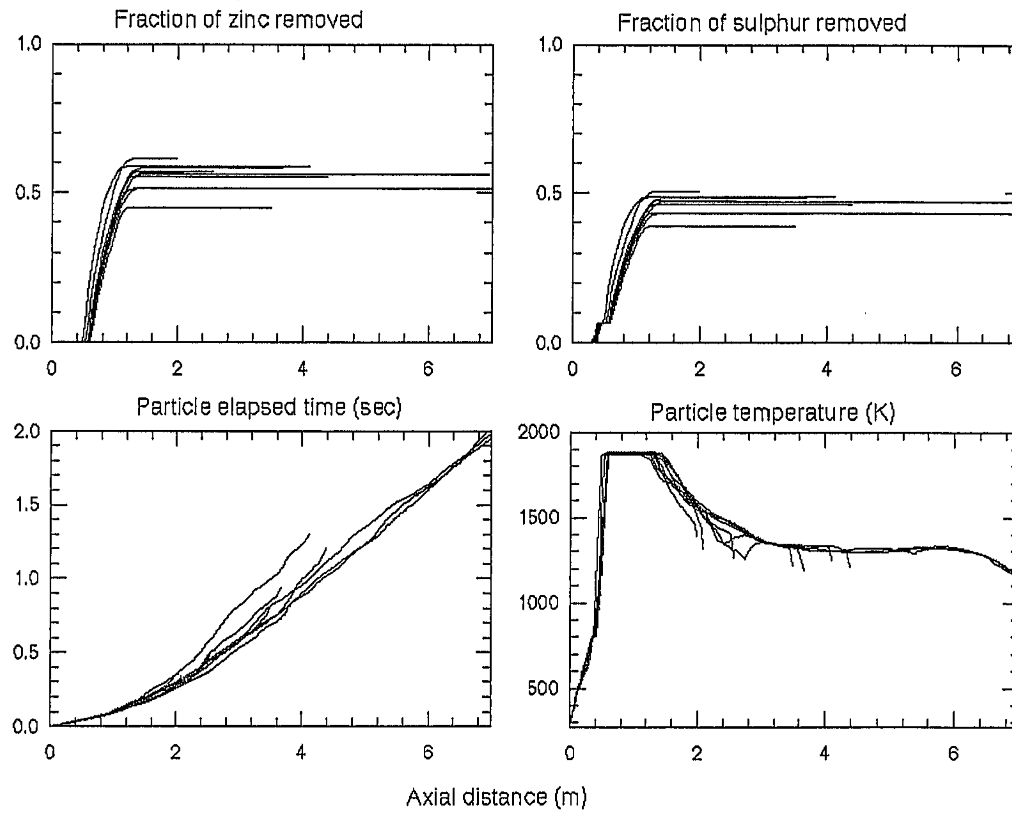

Figure 5. Fractions of zinc and sulphur removed, particle elapsed time and temperature plotted against axial distance from the burner.

The particle tracks and contour plots for a typical case are shown in Figure 4. The particle tracks, shown in side view, are nearly straight with some radial dispersion. The gas flame is long as seen in the fuel contours and some oxygen remains at the bottom of the shaft. Other contour plots in Figure 4 show water vapour, carbon dioxide, sulphur dioxide and zinc vapour that are being produced in the shaft.

Figure 5 shows the particle histories in terms of the fractions of zinc and sulphur removed, particle elapsed time and the particle temperature have all been obtained as functions of axial distance along the shaft. The particle histories indicate that the zinc removal in this simulation is between 45 and 62% and the sulphur removal is less than 50%. The difference between zinc and sulphur is due to the pyrites present in the zinc concentrate. The amount and rate of removal from each solid particle mainly depend on its path and hence the heat transfer and level of oxygen it is exposed to throughout the shaft. The particle residence time is about 2.0 seconds, indicating an average axial velocity of about 3.5 m/s. The corresponding particle temperatures are shown in Figure 5. From an initial temperature of 300K, the particles reach the ZnS decomposition temperature (1873K) within 0.5 m distance from the burner exit.

The zinc volatilizations predicted in this work are conservative as a result of a number of assumptions. For example, it has been assumed that there are no further reactions when the particles hit the wall. In practice, the reactions would continue although at a reduced rate. The formation of solid zinc oxide was not allowed for in the present combustion model. However, it may need to be considered if the model was used in situations where the oxygen concentrations and temperatures in the shaft were different to those encountered in this study.

5. CONCLUSIONS

The zinc flash smelting process has been investigated using a numerical model which combines gas combustion and zinc concentrate combustion. The combined combustion model is a powerful tool which can be used to:

- optimise smelting performance,
- evaluate new burner designs,
- carry out parametric studies, and
- undertake trouble-shooting exercises

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