Design of a three-layer hot-wall horizontal flow MOCVD reactor*

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Abstract: A new three-layer hot-wall horizontal flow metal-organic chemical vapor deposition (MOCVD) reactor is proposed. When the susceptor is heated, the temperature of the wall over the susceptor also increases to the same temperature. Furthermore, the flowing speed of the top layer is also increased by up to four times that of the bottom layer. Both methods effectively decrease the convection and make most of the metal organic (MO) gas and the reactive gas distribute at the bottom surface of the reactor. By selecting appropriate shapes, sizes, nozzles array, and heating area of the walls, the source gases are kept in a laminar flow state. Results of the numeric simulation indicate that the nitrogen is a good carrier to reduce the diffusion among the precursors before arriving at the substrate, which leads to the reduction of pre-reaction. To get a good comparison with the conventional MOCVD horizontal reactor, the two-layer horizontal MOCVD reactor is also investigated. The results indicate that a two-layer reactor cannot control the gas flow effectively when its size and shape are the same as that of the three-layer reactor, so that the concentration distributions of the source gases in the susceptor surface are much more uniform in the new design than those in the conventional one.

Key words: MOCVD; two-layer horizontal reactor; three-layer horizontal reactor; numerical simulation

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1. Introduction

With the increasing application of group-III nitride semiconductors in optoelectronic devices, high quality GaN-based materials, which can work at high temperatures and in some other special conditions, have attracted great attention[1]. High quality material growth techniques such as molecule beam epitaxy (MBE) and metal-organic chemical vapor deposition (MOCVD) were invented to gain high performance devices. However, only the MOCVD technique is able to be applied to the GaN-based material industry due to its large scale production capacity and high material quality[2, 3].

Device performance is mainly determined by the material quality while material quality depends on the flow field and the thermal field. Many high performance MOCVD equipments adopted optimum reactors such as horizontal reactors, vertical reactors, and radial flow reactors. As one of the best radial flow MOCVD reactors, the AIXTRON planetary reactor was first proposed by Frijlink[4] and quickly commercialized due to its large scale production capacity. It is especially suited to the development of the semiconductor industry.

A good reactor should work at a stable laminar state without eddy and distraction near the susceptor. When the material is grown, the reactor should operate under high temperature and low pressure conditions. However, for a conventional MOCVD reactor, only the susceptor is heated to the growth temperature and all other walls are kept at a low temperature with cold water. As a result, there are temperature grads between the hot susceptor and the cooling walls. Thermal convection and thermal diffusion are inevitable[5, 6]. Under these conditions, eddy will be generated and small molecule reactive resource gas will move to the cooling walls and drift in the space. It will then react above the susceptor to form larger molecule particles. When the large molecule particles drop down onto the surface of the susceptor, clusters and cores may be formed, which is harmful to the film quality. If the temperature grads could be weakened, the thermal convection could be reduced drastically. From our simulation and experimental results, using a hot wall MOCVD reactor is a good method. It means that the reactor wall is kept at a relatively high temperature and even up to the same temperature as the susceptor[7−9].

In our paper, we give a new design of a three-layer hot-wall horizontal flow MOCVD reactor. By heating some necessary walls, except for the susceptor, the thermal convection towards the top wall is effectively decreased. Most of the source gases localize on the surface of the susceptor in a steady laminar flowing state and the density of the reactive resource gases is much higher than that of the top wall. To gain a deep contrast with the conventional cold-wall MOCVD reactor, the two-layer horizontal MOCVD reactor is also studied in detail and both results are compared, which indicates that a conventional reactor cannot control the gas flow effectively. It can be inferred that the three-layer hot-wall reactor achieves an advantage over the conventional two-layer reactor and has good prospects for the future. Although the horizontal reactor has a relatively small production capacity compared with the high production capacity of a multi-wafer vertical reactor, it has a more homogeneous resource gas distribution. In the vertical

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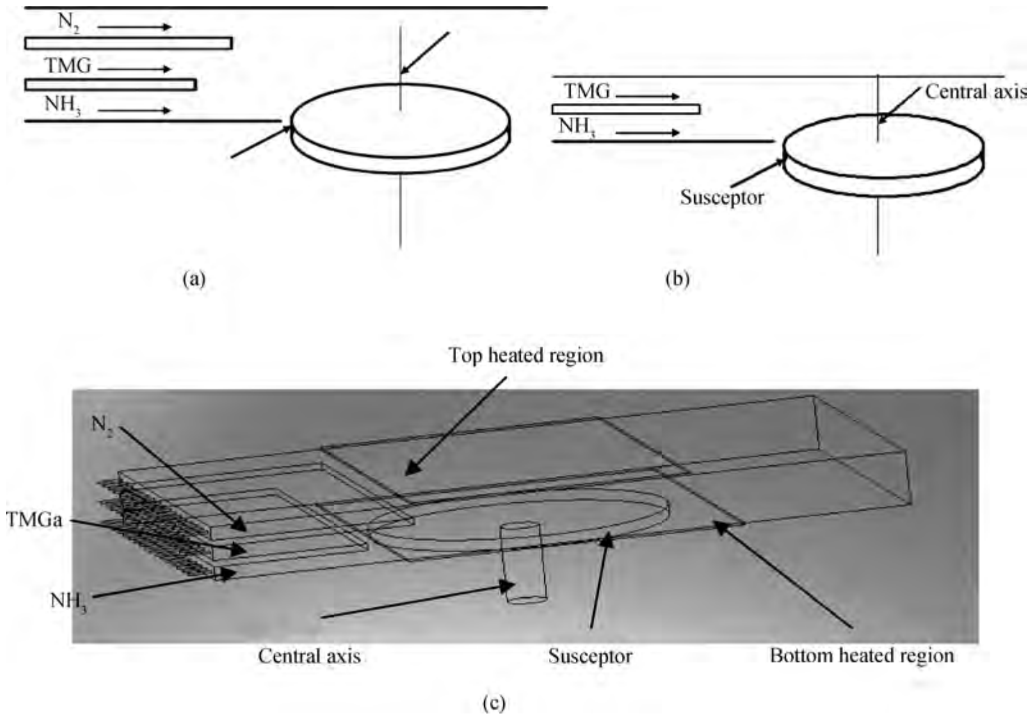

Fig. 1. The whole structural diagram of (a) the three-layer MOCVD reactor and (b) the conventional two-layer cold-wall MOCVD reactor. The detailed structure of the three-layer hot-wall MOCVD reactor is shown in (c), which can decrease the thermal convection around the susceptor by heating the top and bottom walls.

MOCVD reactors, there still exists weak convection even if the resource flows downwards to the susceptor. And if the hot-wall technique can be applied to vertical reactors, it can improve the material quality significantly.

2. Model description

The three-layer hot-wall MOCVD reactor and the conventional design are given in Figs. 1(a) and 1(b), respectively. The 3D structure of the three-layer reactor is also shown in Fig. 1(c). Our design consists of three 6.3-mm-thick horizontal layers separated by two 3-mm-thick baffles, the lengths of which are 84 mm and 64 mm, respectively. The total length of the reactor is 289 mm. The diameter of susceptor is about 122 mm and the upper edge of the susceptor is 20 mm away from the end of the lower baffle. In addition to above geometry parameters, there are two rectangular heated regions. One is on the top layer (170×120 mm^2) and the other is in the bottom surface around the susceptor (170×140 mm^2). Both of the temperatures are the same as the susceptor in order to reduce the convection between the two walls. The NH_3, trimethyl gallium (TMGa), and N_2 enter into the reactor from the respective 17 jets, the diameters of which are all 1 mm. The source gases flow forwards under the parallel jet states. When they arrive at the susceptor surface, the chemical reaction will occur and the exhaust will flow away from the surface. All the parameters of the conventional reactor are the same as our new design except for the two layers shown in Fig. 1(b). To simplify the physical model and describe the flow as accurately as possible, the following assumptions are made.

(1) The reactor is in a steady flowing state.

(2) The susceptor and the rectangular heated regions are heat sources and it radiates different heat fluxes from different places on the surface, therefore the temperature in the surface is different between the center and the outer edges.

(3) The TMGa and the carrier gas are mixed equably.

(4) The walls of the reactor are not adiabatic.

(5) The MOCVD reactor is filled with N_2 at a pressure of 76 Torr and during the growth, N_2 works as carrier gas.

(6) The flow flux of the source gases, namely NH_3 and trimethyl gallium (TMGa), entering into reactor is 1 SLM, and the flow flux of the carrier, namely N_2, is 4 SLM.

As the reactant concentrations are much smaller than the precursor's and the effect on the fluid state is very weak, the chemical reactions could be neglected. In order to overcome the problem that the precursor concentration distribution is different along the longitudinal direction on the surface, the susceptor rotates around its central axis at a constant speed of 30 r/min. Since the flowing speed in the reactor is very slow, the fluidity is assumed as incompressible gas and the velocities are specified in the inlets. The "pressure outlet" boundary conditions are named and there is fully developed flow at the outlet. The reactor is a pressure-velocity coupling field. The parallel jet has complicated turbulence and needs to be solved by using the default SIMPLE algorithms method.

3. Numerical simulation results

The source gases' concentration distributions 0.5 mm above the susceptor surface of the reactor are shown in Fig. 2, in which the flowing direction of the gases is along the z axis. The concentrations of NH_3, TMGa and N_2 in the three-layer hot-wall reactor are shown in Figs. 2(a), 2(b), and 2(c), while the corresponding concentrations in the two-layer reactor are

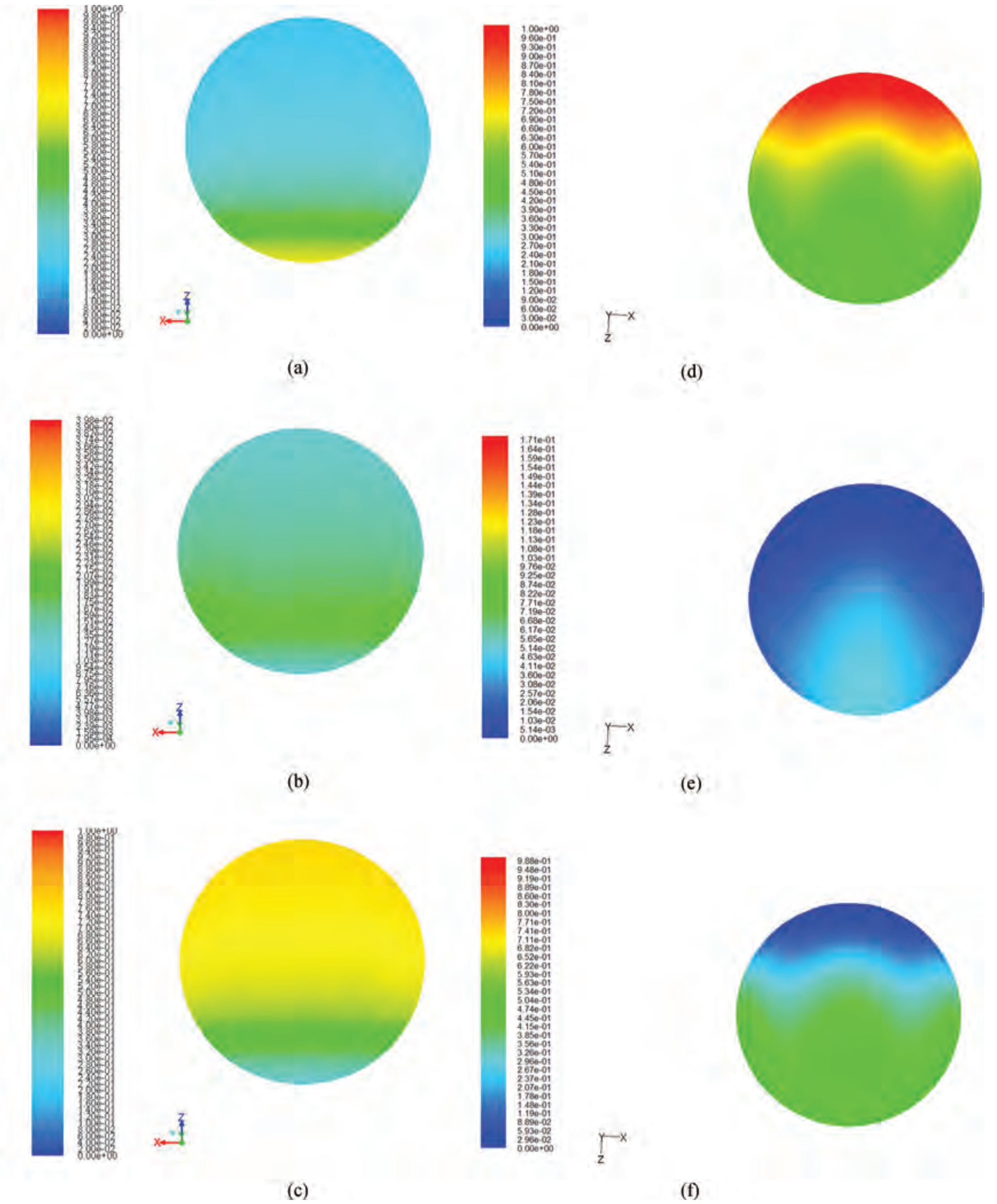

Fig. 2. (Color online) The concentration distributions of NH_3, TMGa, and N_2 on the susceptor of the three-layer hot-wall reactor are shown in (a), (b), and (c). The corresponding concentrations in the two-layer reactor are given in (d), (e), and (f).

shown in Figs. 2(d), 2(e), and 2(f), respectively. It indicates that the concentrations of NH_3, TMGa, and N_2 are very uniform except at the brims of the susceptor. The corresponding concentrations in the conventional reactor are not so uniform. As is well known, a little uniformity at the edge of the susceptor hardly affects the quality of the materials because the materials are grown mainly in the central part. The TMGa concentration distribution is not very uniform and when the susceptor rotates around its central axis at a certain speed, this problem can be overcome.

Overall, the concentration distributions in the three-layer hot-wall reactor are more uniform than those in the two-layer reactor. One of the reasons is that it is helpful for the three-layer reactor to reduce the pre-reaction between the precursors due to the different size of the upper and the lower baffle. Secondly, the high speed N_2 flow in the top layer contributes to reduce the thermal convection of the reactants above the substrate and the deposition on the upper reactor wall. However, the results of the two-layer reactor are opposite to that of the three-layer reactor. Therefore, the precursors in the three-layer reactor can flow in a relatively steady velocity and the composition of the precursors is also able to keep relatively uniform at the same time so that the concentration distributions in the three-layer reactor are more uniform.

The velocity vector field, including partial magnification around the susceptor for the central planes along the flowing

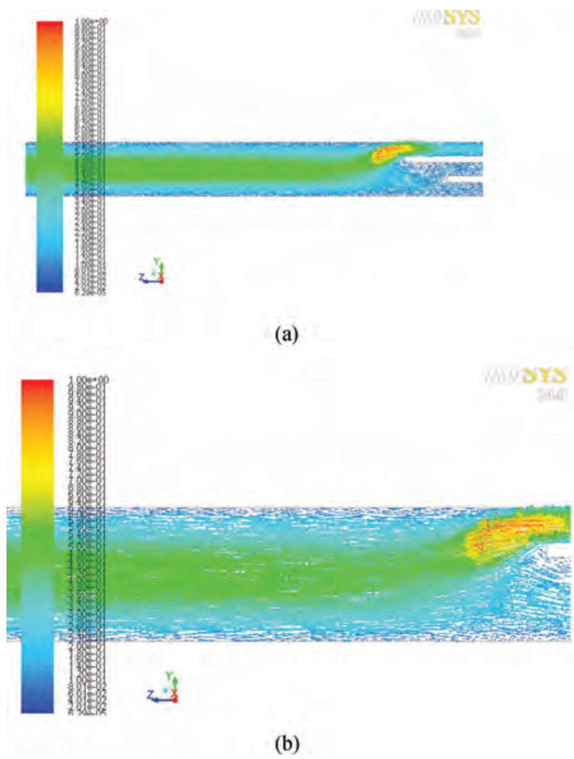

Fig. 3. (Color online) The diagram of (a) the velocity vector and (b) its partial magnification near the susceptor of the three-layer hot-wall MOCVD reactor. No eddy and backflow can be seen in the reactors and the velocity distribution is homogeneous.

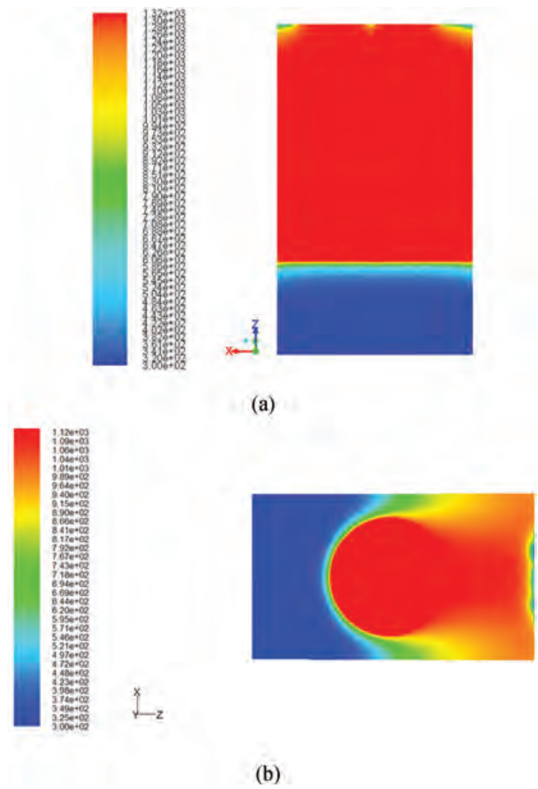

Fig. 4. (Color online) The temperature field of (a) the three-layer hot-wall MOCVD reactor and (b) the two-layer cold-wall MOCVD 0.5 mm above the susceptor surface. It is very evident that the former temperature distribution is more uniform than that of the latter.

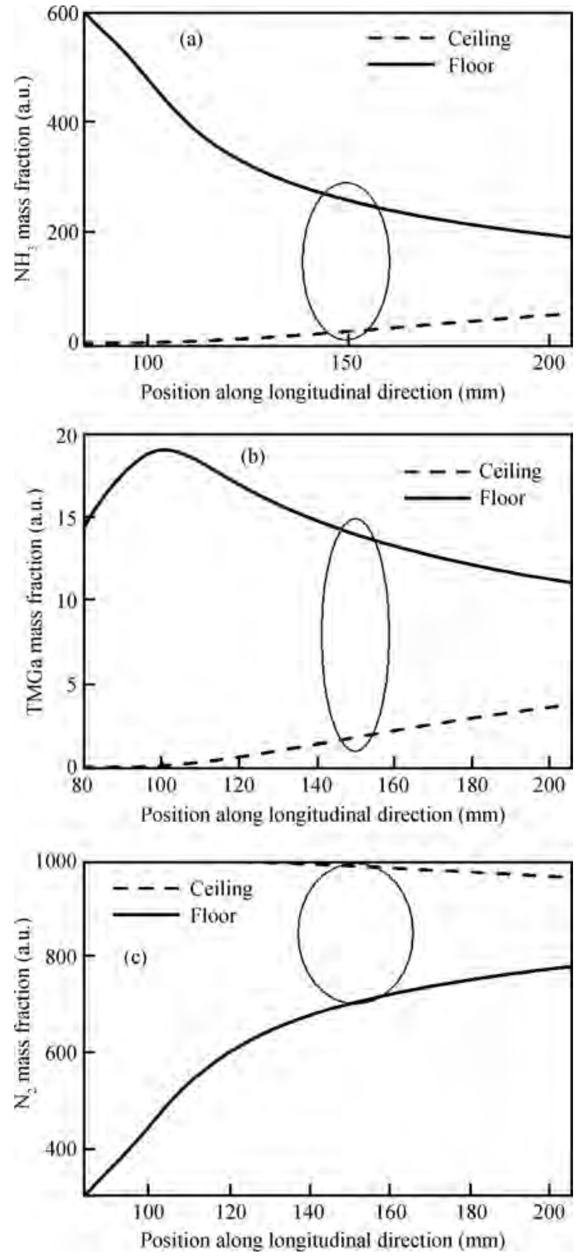

Fig. 5. The source gas concentration (a) NH_3, (b) TMGa and (c) the carrier gas concentration N_2 on the top wall surface and the bottom wall surface.

direction in the three-layer reactor, is shown in Fig. 3. No eddy or backflow can be seen in the whole structures although there is a difference among the different parts. In addition, the growth of the samples in our design is only localized at the bottom part, where flowing is relatively slow and more homogeneous. As shown in Fig. 5, it can also be concluded that there are only a small changes of the mass fraction of the central part marked with the circle. At the same time, the susceptor rotates around its central axis at a certain speed. Therefore, the difference in velocity hardly affects the quality of the materials.

The thermal temperature field 0.5 mm above the susceptor surface, corresponding to the thickness of the substrates, and its neighboring environment are shown in Fig. 4(a) for the new design and the corresponding conventional one are shown in Fig. 4(b). It is evident that the susceptor surface and the adjacent surface of the three-layer hot-wall MOCVD reactor are more uniform and it is of benefit to the material growth. The temperature in the susceptor of the conventional reactor is also uniform, but the change of the temperature at the edge of the susceptor is very sharp. Sometimes the thermal convection and the small eddy are inevitable, which will harm material growth.

The mass fraction of NH_3, TMGa, and N_2 in the susceptor surface and the top hot-wall along the longitudinal direction is shown in Figs. 5(a), 5(b), and 5(c), respectively. The top-wall surface is represented as 'Ceiling' while the bottom wall surface is represented as 'Floor'. For the three-layer hot-wall MOCVD reactor, it is clear that the concentration of the source gas in the bottom wall surface is much higher than that in the top wall surface, by at least three or five times. It indicates that the thermal convection is decreased greatly in the hot-wall reactor. Although the two walls are the same temperature as the susceptor's, the carrier gas and source gases are cold. As a result, there are temperature grads between the walls and the central space where the gas flows through. One method is adopted to solve this problem. The heated rectangular region is enlarged enough in order to insure that the gas is heated up to the same temperature as the hot-wall before arriving at the susceptor. The concentrations along the longitudinal direction are not the equal, but the susceptor will rotate around its central axis, which can compensate the unbalance. Furthermore, the material growth is almost in the central part of the susceptor, and the concentration fluctuation is relatively low. It will be very desirable to improve the uniformity of the thickness and the component for the grown film. The results shown in Fig. 5 are consistent with that shown in Fig. 2. According to above source gas distribution, the chemical vapor deposition will mainly focus on the susceptor surface. The fraction of the deposition on the top wall is relatively very weak. To our knowledge, this is the first time that a three-layer hot-wall MOCVD reactor has been proposed. It will decrease convection effectively.

4. Conclusion

In summary, a new three-layer hot-wall horizontal MOCVD reactor has been proposed. It can decrease the thermal convection by heating the top wall up to the same temperature as the susceptor. The concentration distribution of the reactants on the susceptor surface was simulated by using CFD simulation with FLUENT software. The concentration distributions of NH_3, TMGa, and N_2 0.5 mm above the susceptor surface in the three-layer hot-wall reactor are much more uniform than that in the conventional two-layer reactor. No eddy or backflow in the whole structure could be seen and the temperature in the susceptor surface, including its adjacent hot-wall reactor regions, is more desirable for material growth than in a conventional reactor. It indicates that three-layer hot-wall reactor has a better performance than the conventional design. It is the first time that a three-layer hot-wall MOCVD reactor has been simulated and it is a realizable technique to decrease the convection. Though the horizontal three-layer hot-wall reactor has a low production capacity compared with the multi-wafer vertical reactor, it has a more stable flowing state. If the hot-wall technique is applied to the vertical reactor, the material quality can be improved to a large extent.

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