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Mathematical Modelling of Complex Flow Phenomena in Vertical Chemical Vapour Deposition Reactors

1. Introduction

Since convection and diffusion regulate the transport of heat and species, fluid flow phenomena strongly influence the chemical vapor deposition (CVD) process in electronic material fabrication. This fact explains the considerable interest in investigation of flow structures in CVD reactors.

In this work selected results of numerical simulation of convective heat transfer for various vertical CVD reactors are presented with emphasis on their effect on the non-uniformity of epitaxial layer thickness and composition. Thermodynamic data for chemical kinetics are not available for these processes. The growth conditions of the above reactors correspond to the diffusion-limited deposition. Hence, in that case it is possible to analyze growth properties by making use of the heat and mass transfer analogy without the individual species transport consideration.

2. Reactor model

Reactor design is important because of its strong influence on the uniformity of the deposition and the ability of forming abrupt interfaces. High-capacity reactors are generally of the "barrel" design, in which the substrates are placed almost vertically on a barrel-shape susceptor [1]. The susceptor is rotated to improve deposition uniformity.

The complete growth process including chemical, thermal and hydrodynamic effects is extremely complex and hence difficult to model accurately [2]. The simple conception of a concentration and thermal boundary layer is not sufficient for the accurate modelling of the fluid-thermal environment in the reactors. So, assuming the uncoupling of the hydrodynamic problem from mass transfer, we will consider the following model to analyze the structure of convective heat transfer in vertical CVD reactors.

The transport of heat and momentum for axisymmetric incompressible flow is governed by 2D Navier-Stokes equations in the vorticity-stream function formulation with Boussinesq approximation for buoyancy:

$$\frac{\partial T}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(ruT) + \frac{\partial}{\partial z}(vT) = \frac{1}{Pr \cdot Re}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] \qquad (1)$$

$$\frac{\partial \omega}{\partial t} + \frac{\partial}{\partial r}(u\omega) + \frac{\partial}{\partial z}(v\omega) = \frac{1}{Re}\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(r\omega)\right) + \frac{\partial^2 \omega}{\partial z^2}\right] - \frac{Gr}{Re^2}\frac{\partial T}{\partial r} \qquad (2)$$

$$\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial \psi}{\partial r}\right) + \frac{1}{r}\frac{\partial^2 \psi}{\partial z^2} = -\omega , \quad u = -\frac{1}{r}\frac{\partial \psi}{\partial z} , \quad v = \frac{1}{r}\frac{\partial \psi}{\partial r} \qquad (3)$$

Here T, ω, ψ, u and v are dimensionless temperature, vorticity, stream function, radial and axial velocities, respectively; r is the radial coordinate and z is axial coordinate. Pr, Re and Gr are Prandtl, Reynolds and Grashof numbers, respectively.

The boundary conditions used in our predictions for all CVD reactors are:

- no slip, no permeability condition on susceptor and reactor walls;
- experimentally measured susceptor and wall temperature profiles;
- zero radial derivatives of temperature and fixed zero values of vorticity and stream function on the symmetry axis;
- developed or uniform inlet velocity profile with given gas temperature and volumetric flow rate;
- zero axial derivatives of temperature, vorticity and stream function at the outlet.

The set of coupled equations (1)-(3) was solved numerically with the above mentioned boundary conditions using finite difference code NEPTUNE [3]. A rectangular grid with a non-uniform spacing, used in complex flow domain calculations, was finer near the susceptor and walls and coarser elsewere. Grid with about 1500 points was found appropriate for the accuracy of the solution and the cost of the calculations. Two grids used in the calculations are depicted in Fig.4.

3. Results and discussions

Three various kinds of vertical CVD reactors have been considered for typical operating conditions. Two of them fabricate GaAs (metalorganic CVD) and the third deals with chloride compounds production.

Large thermal gradients can generate buoyancy driven secondary flows which produce a negative influence on the film deposition rate and composition. To suppress such zones of recirculation near of susceptor by means of suitable reactor geometry and operating conditions - that is the aim of all our calculations.

The first considered MOCVD reactor (Fig.1) have a pyramidal base with a small inclination angle for substrates and a down flow inlet. Strong buoyancy driven cell above the susceptor exist in reactors of similar geometry [4]. It was found in predictions that the small size of the annulus between susceptor surface and reactor wall and a high volumetric flow rate can eliminate secondary flows near the susceptor and create forced convection regime. The circular arc shape of the top wall has reduced but not eliminated the recirculations.

The second MOCVD high-capacity reactor (Fig.3) had similar construction as considered in [5]. Large secondary cells exist near the vertical susceptor in such flow configuration. An opposite injection direction - upflow inlet - has been proposed to remove the secondary cell from susceptor to the reactor wall.

Three inlets with different gas temperatures and volumetric flow rates are used for chloride compounds production (Fig.2). Despite of the two buoyancy driven cells at the upper part of the reactor chamber, such a complex flow configuration provides enough uniformity of the flow structure near the susceptor.

The present numerical simulations demonstrate that wall effects, susceptor heating and secondary flows may lead to a reducion of the quality of the produced materials.

References

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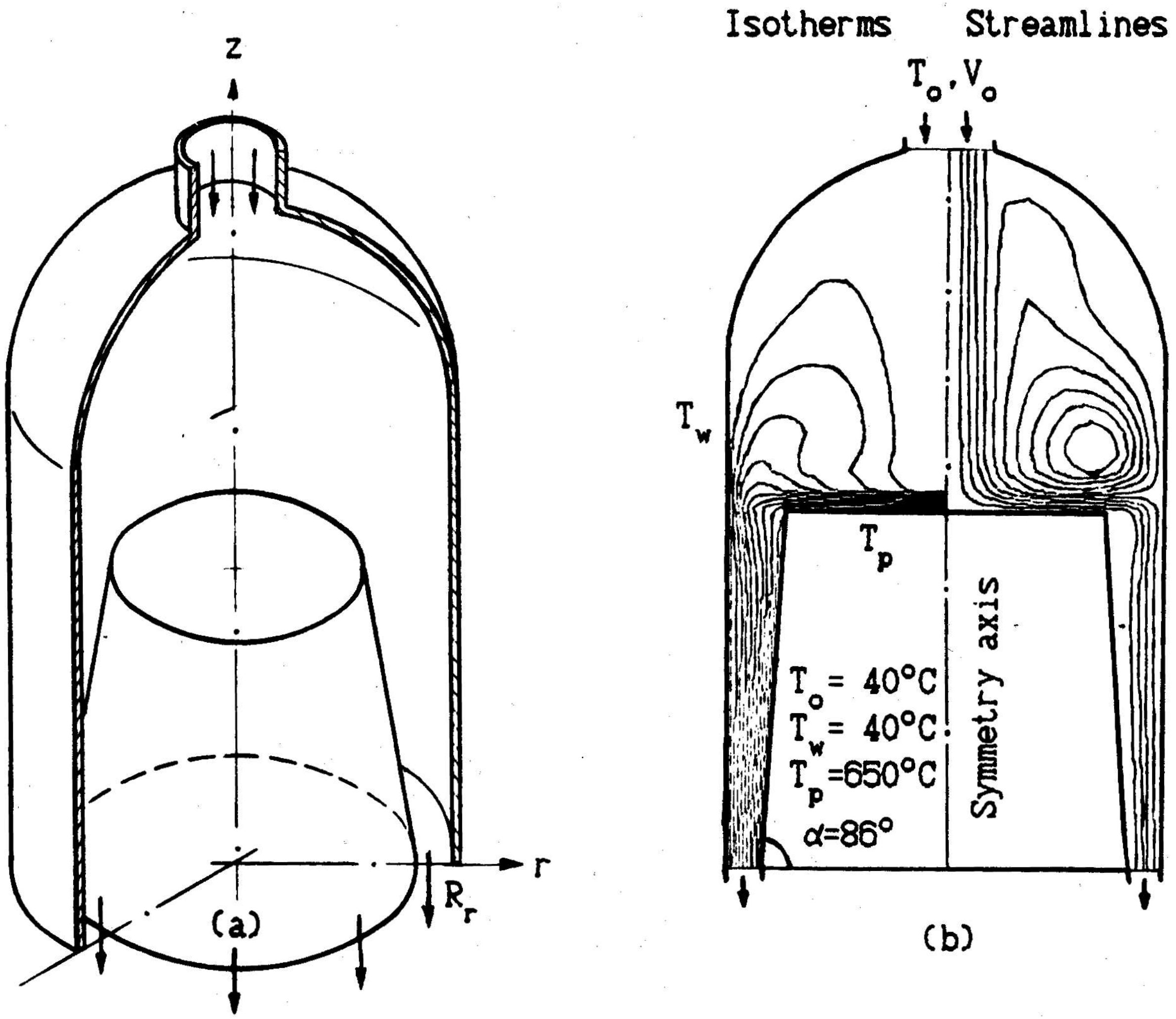

Fig.1 Calculation of mixed convection in chemical vapour deposition reactor with pyramidal base: (a) sketch of reactor; (b) temperature field and gas flow pattern for $Re = V_o R_r / \nu = 90.$ and $Gr/Re^2 = 4.5$

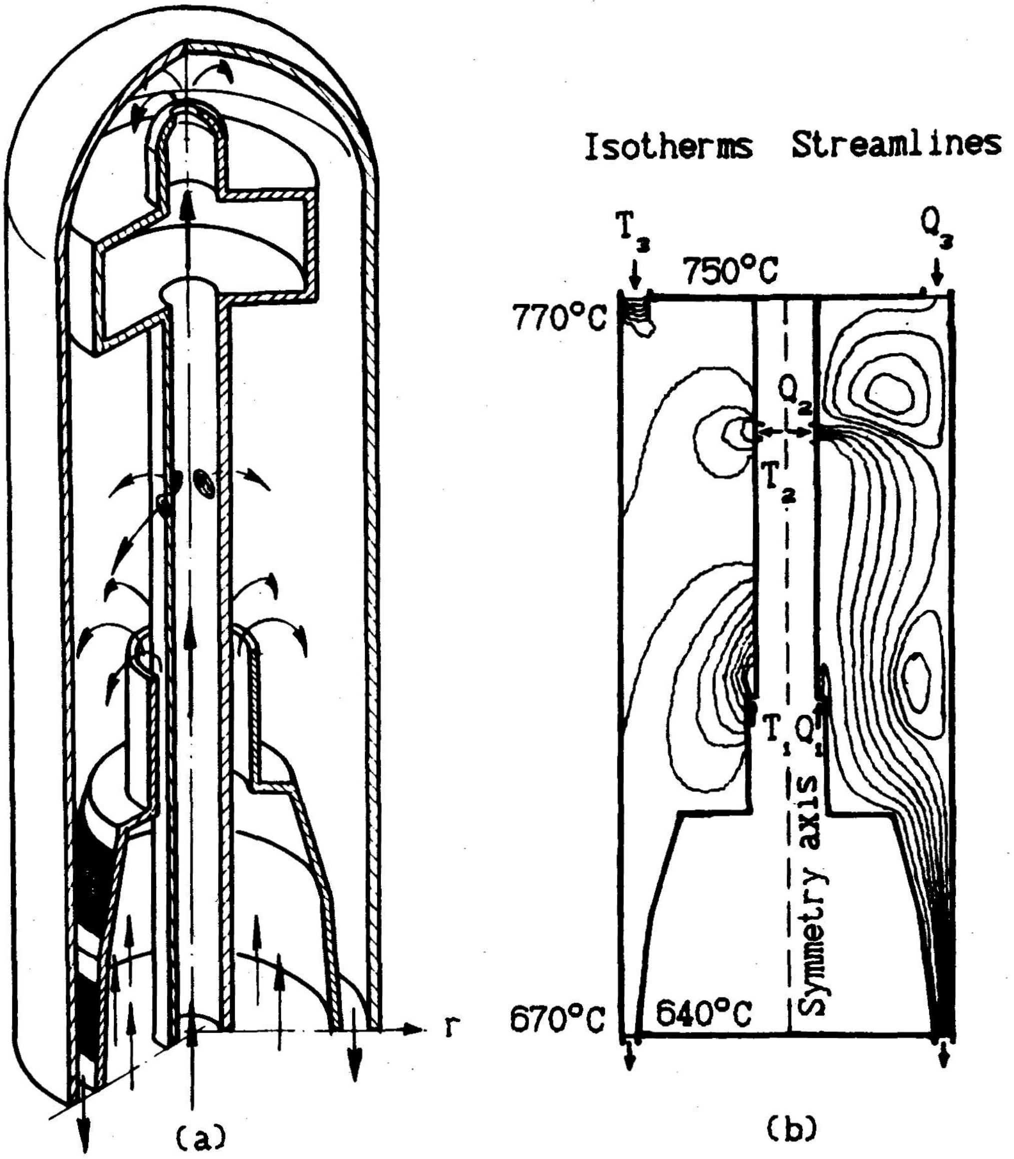

Fig.2 Modelling of pas-epitaxial reactor for chloride compounds production: (a) sketch of reactor; (b) calculated mixed convection for three inlets with different temperatures and flow rates for Re = 5.4, $Gr/Re^2 = 103$,

$T_1 = 300^0C$, $T_2 = 360^0C$, $T_3 = 400^0C$

$Q_1 = 0.040 \times Q_\Sigma$, $Q_2 = 0.933 \times Q_\Sigma$ $Q_3 = 0.027 \times Q_\Sigma$

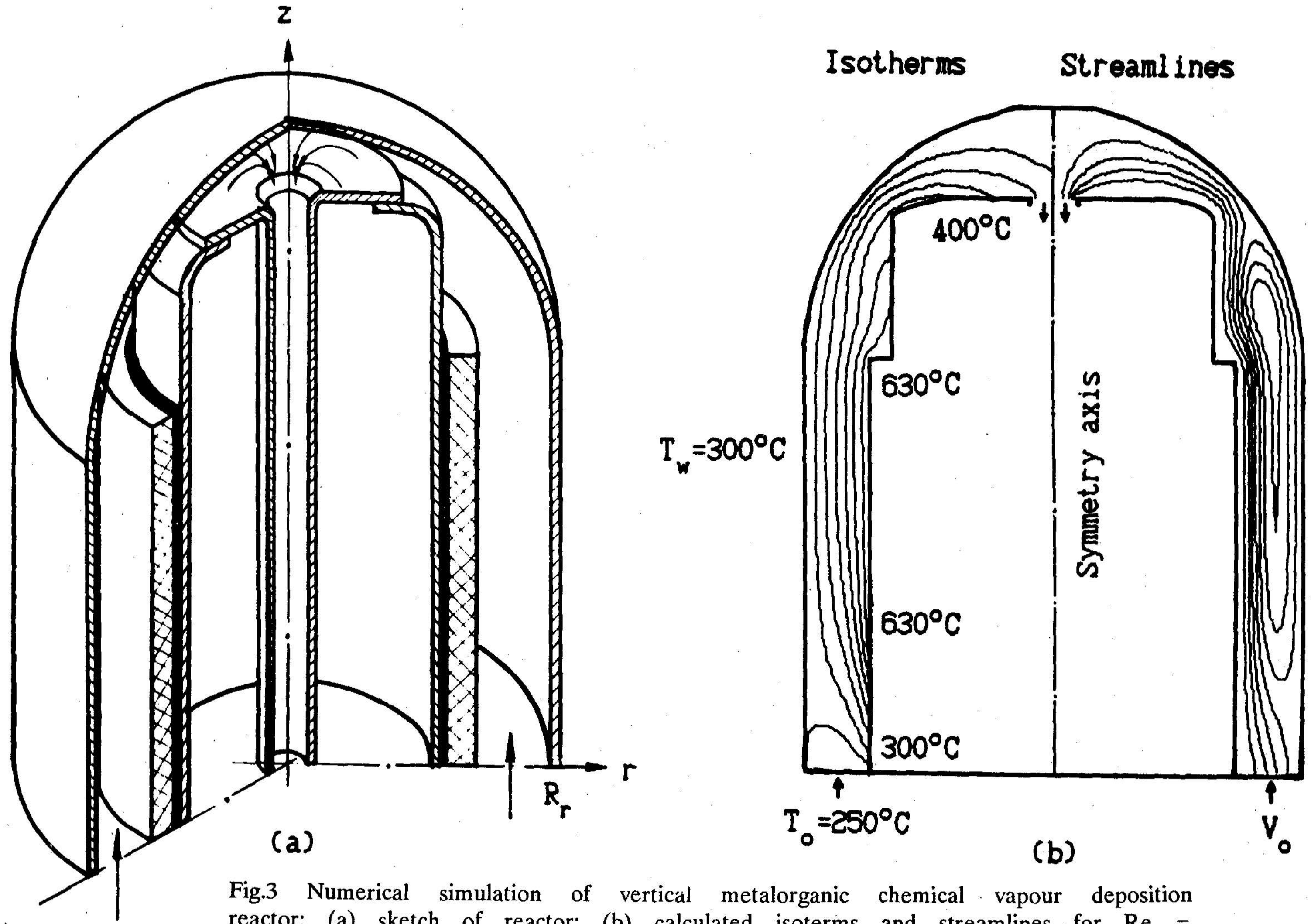

Fig.3 Numerical simulation of vertical metalorganic chemical vapour deposition reactor: (a) sketch of reactor; (b) calculated isoterms and streamlines for $Re = V_0 \times R_r / v = 17$, $Gr/Re^2 = 380$.

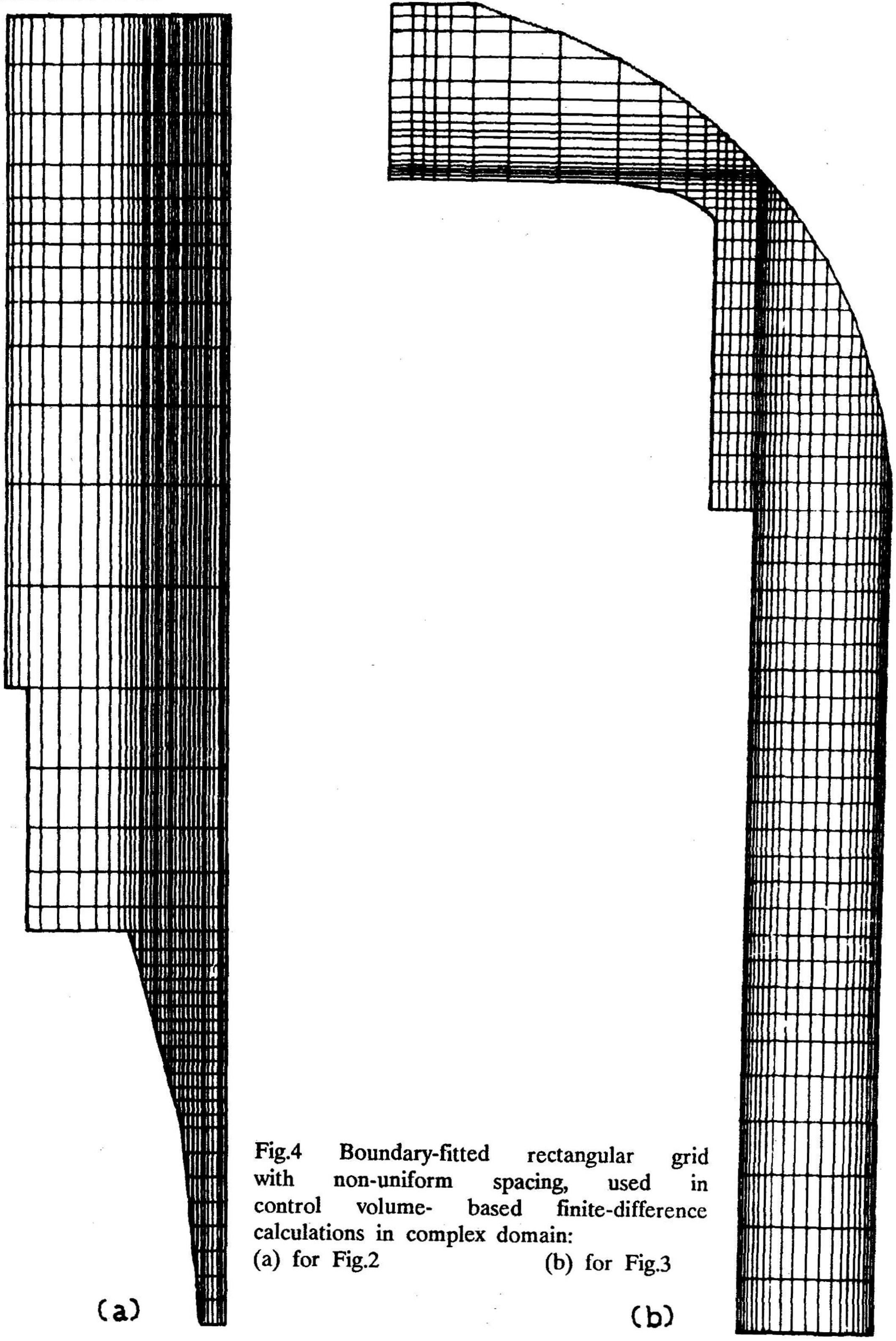

Fig.4 Boundary-fitted rectangular grid with non-uniform spacing, used in control volume- based finite-difference calculations in complex domain:
(a) for Fig.2 (b) for Fig.3