Numerical Simulation of MOCVD Growth of Semiconductor Compounds

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Contents

- Simulation output.
- Fluid flow and heat transfer models.
- Gas and surface reactions models.
- MOCVD reactor models.
- Example of GaAs growth.
- Example of GaN growth.
- Rotating disk model.

Simulation output

- Chemical species distributions in reactor.
- Gas flow pattern.
- Temperature distribution.
- Film deposition rates and composition.
- Common impurity incorporation.

Fluid Flow

1. Continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho V)$$

2. Momentum conservation

$$\frac{\partial (\rho V)}{\partial t} = -\nabla \cdot (\rho V V) + \nabla \cdot \tau - \nabla P + \rho g$$

Heat and Species transfer

3. Energy Conservation

$$\frac{\partial (c_p \rho T)}{\partial t} = -\nabla \cdot (\rho c_p V T) + \nabla \cdot (\lambda \nabla T)$$

4. Species Transport

$$\frac{\partial (\rho \omega_i)}{\partial t} = -\nabla \cdot (\rho V \omega_i) - \nabla \cdot j_i + S_i$$

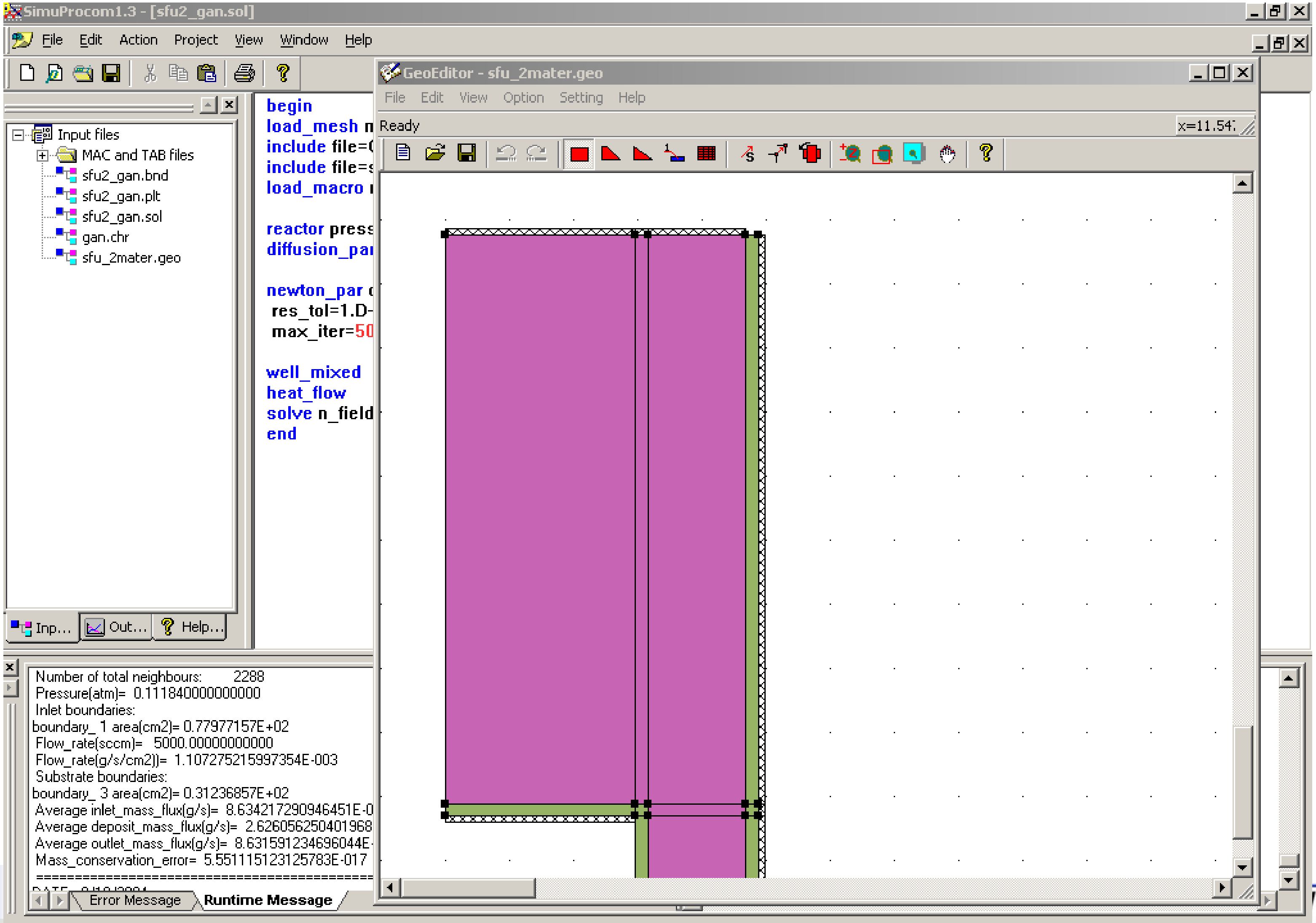
Gas and Surface Reactions

- Detailed gas phase reaction models for GaAs, InP, InGaAsP, GaN and AlGaN materials.
- Precursors: TMGa, TMAl, TMIn, TEGa, TBAs, NH3, AsH3, TBP ...
- Well calibrated surface reaction models for GaAs, InP, InGaAsP, GaN and AlGaN materials.

Built in Reactor Models

- Horizontal reactor
- Vertical reactor
- Planetary reactor
- Barrel reactor

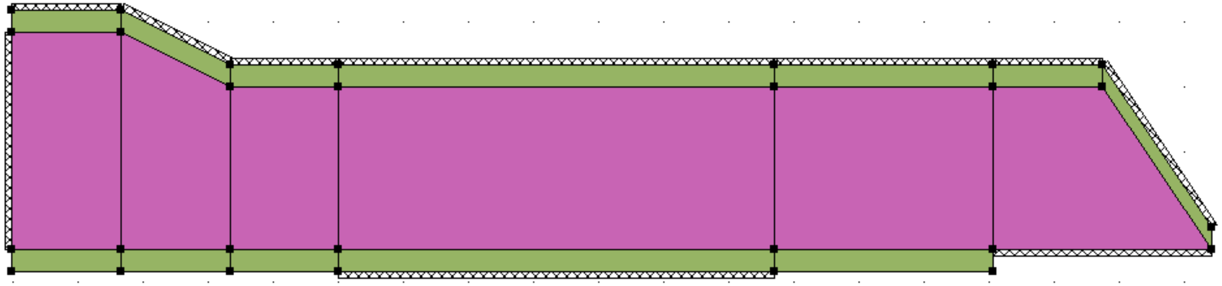
User Friendly GUI

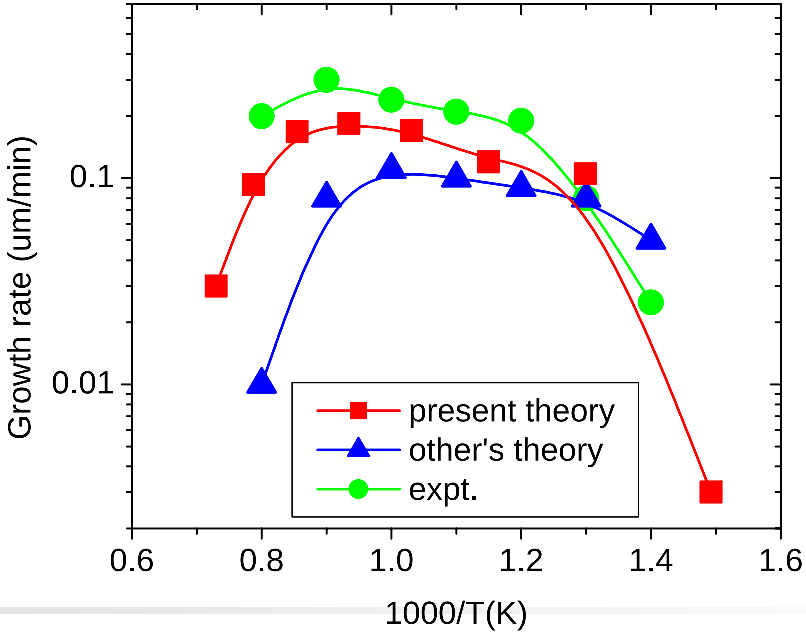


```
begin
load_mesh
include file=
include file=
load_macro

reactor press
diffusion_pa

newton_par
 res_tol=1.D-
 max_iter=50

well_mixed
heat_flow
solve n_field
end
```

```
 Number of total neighbours:      2288
 Pressure(atm)=  0.111840000000000
 Inlet boundaries:
boundary_ 1 area(cm2)= 0.77977157E+02
 Flow_rate(sccm)=   5000.00000000000
 Flow_rate(g/s/cm2))=  1.107275215997354E-003
 Substrate boundaries:
boundary_ 3 area(cm2)= 0.31236857E+02
 Average inlet_mass_flux(g/s)=  8.634217290946451E-0
 Average deposit_mass_flux(g/s)=  2.626056250401968
 Average outlet_mass_flux(g/s)=  8.631591234696044E
 Mass_conservation_error=  5.551115123125783E-017
 ======================================================
```

GaAs Growth in Horizontal reactor





Growth rate vs. temperature

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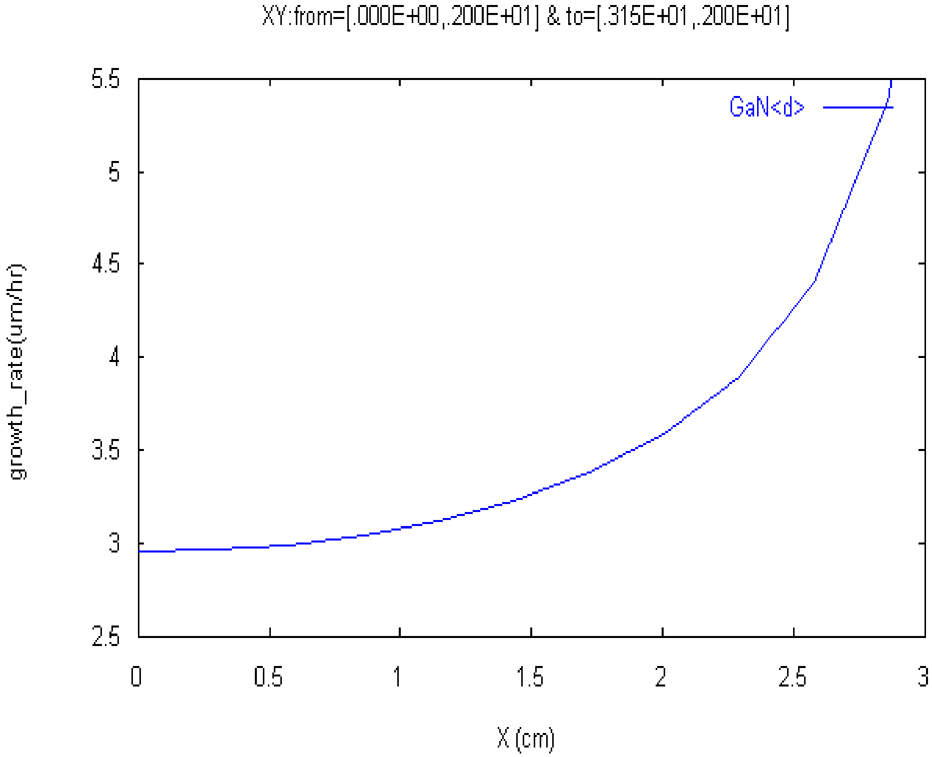
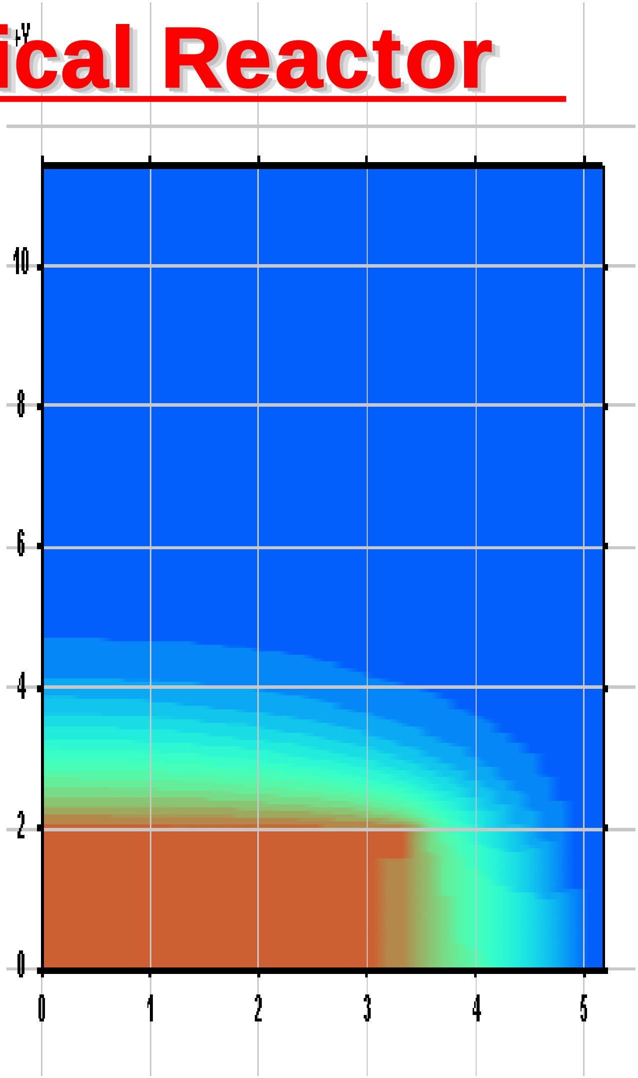
GaN Growth in Vertical Reactor

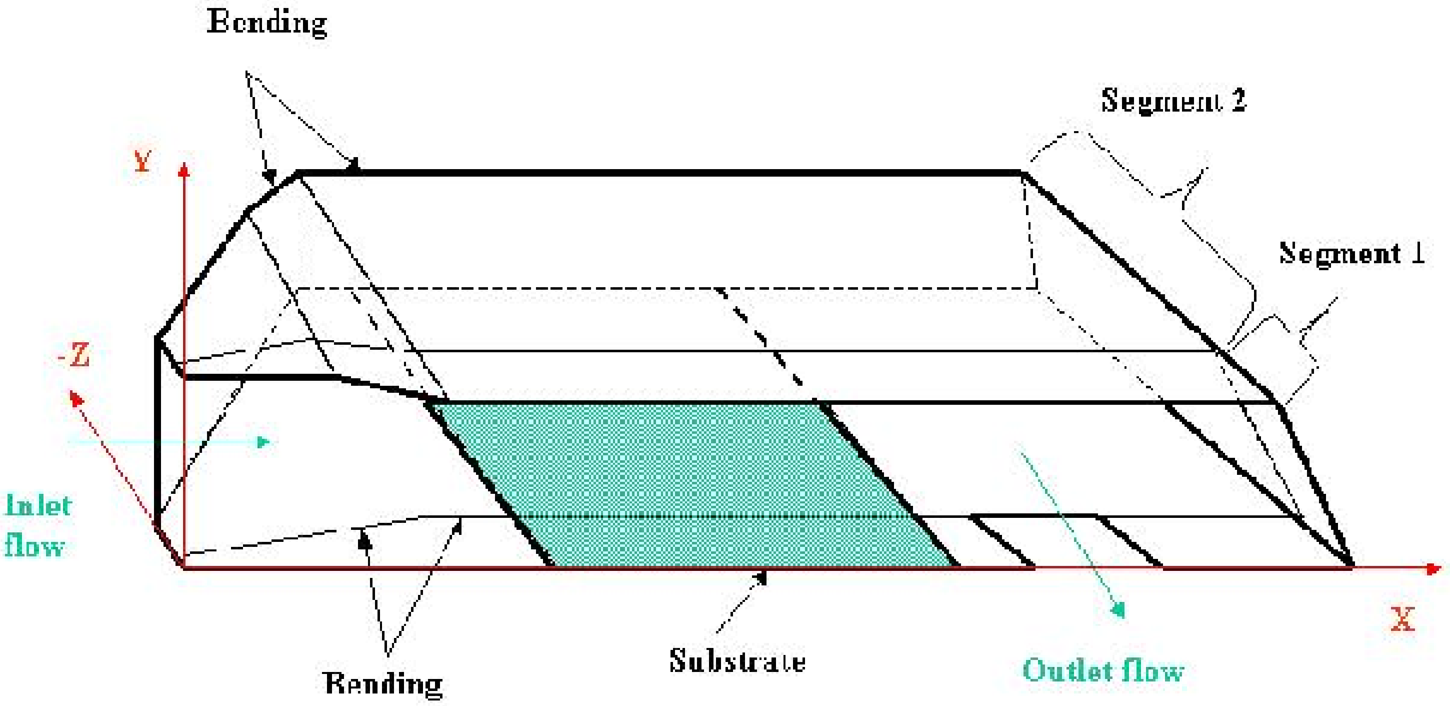


Growth rate vs. position on substrate



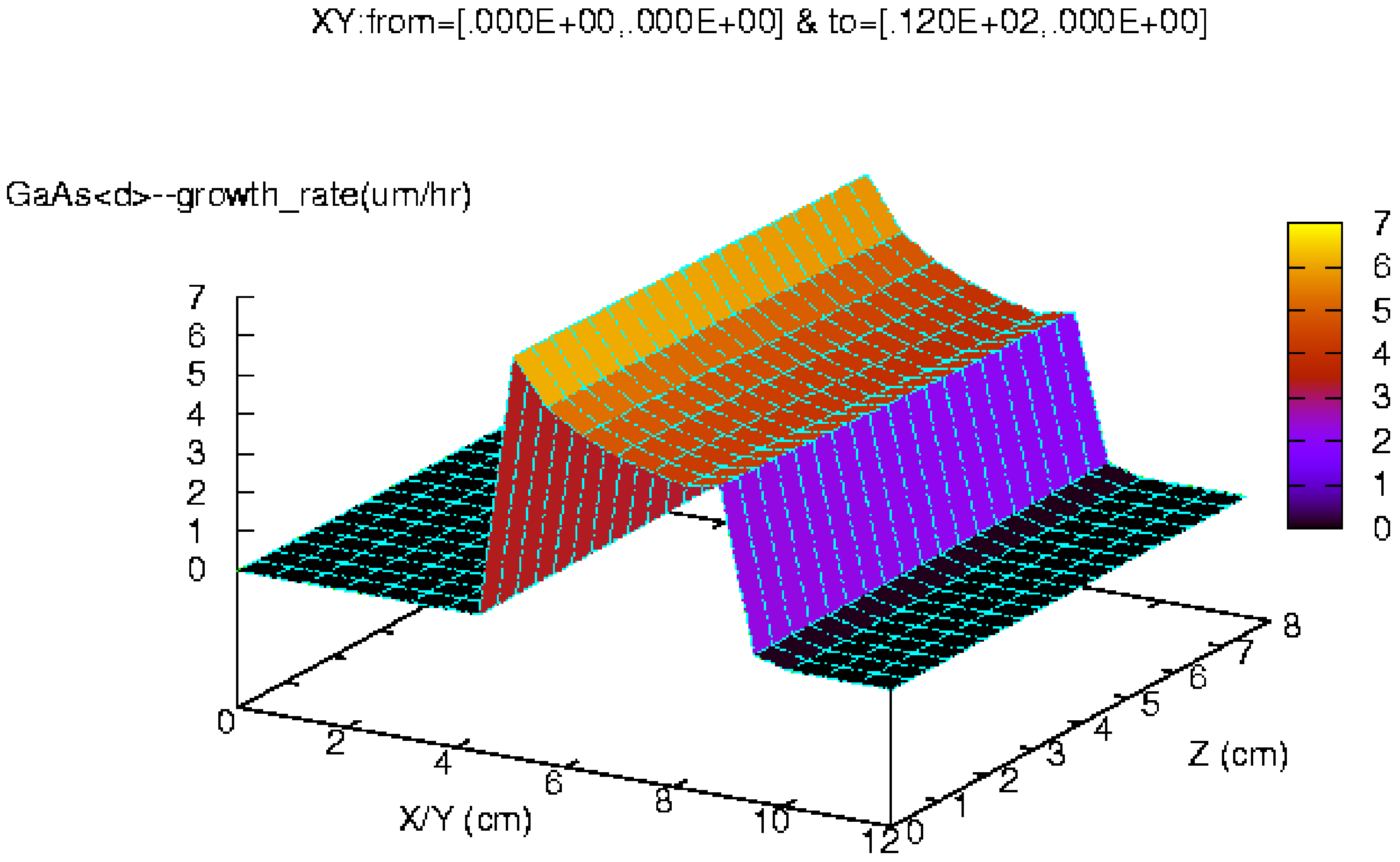
Temperature distribution in reactor

3D Simulation of GaAs Growth in Horizontal Reactor



Reactor model in 3D, only half of it is shown because of symmetry of the reactor

GaAs Growth Rates in 3D



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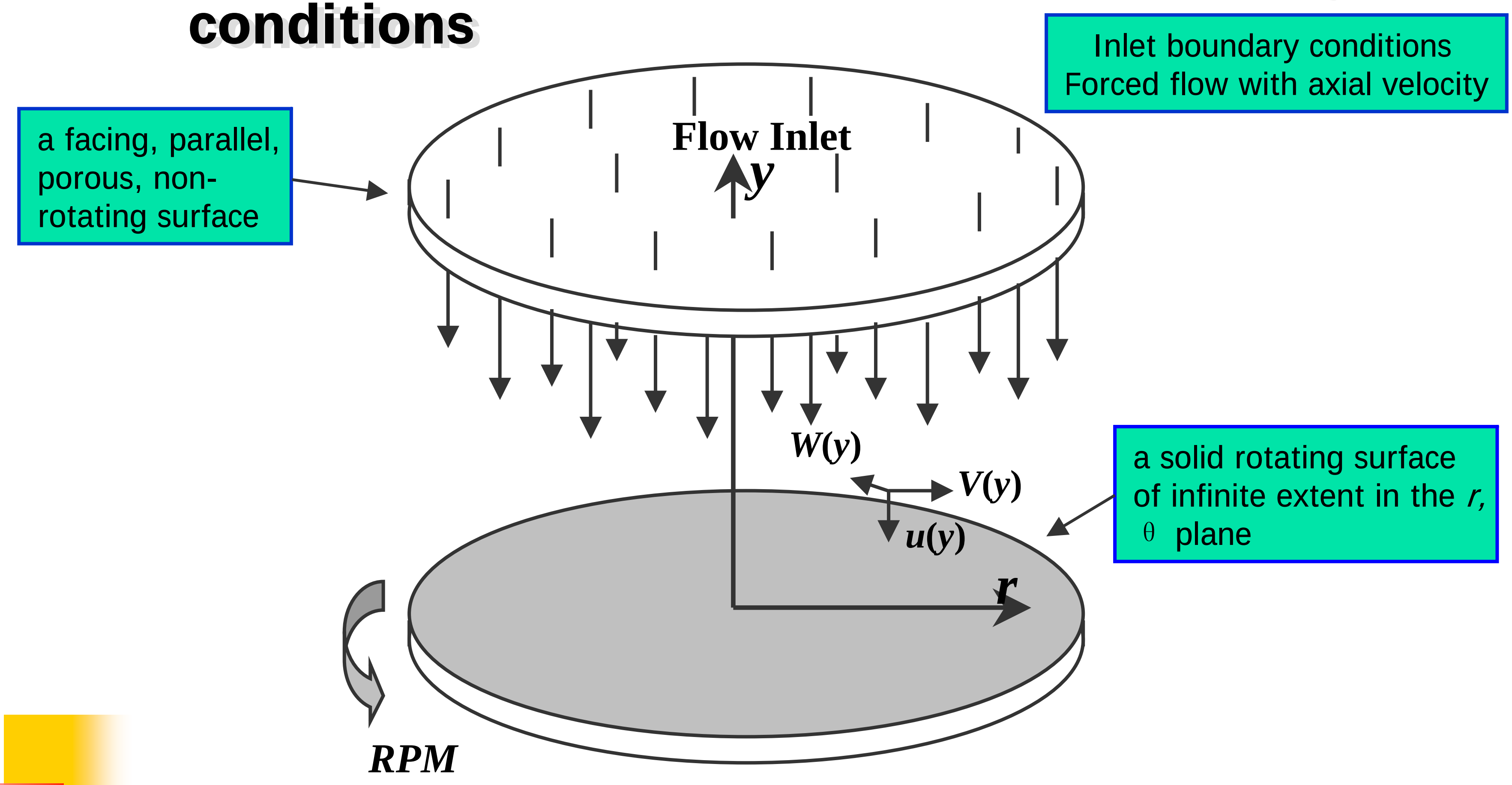
Introduction

- Rotating disk has great potential for highly uniform film growth.
- Commercial rotating disk reactors are common.
- PROCOM uses a variable separation transformation to obtain good practical approximation for efficient gas flow solutions.
- PROCOM combines rotating disk solution with chemical reaction, mass transport, heat transfer and multiple gas inlet boundaries models.

Simplified boundaries for fuild flow

- **the infinite-radius disk and inlet boundary conditions**



Inlet boundary conditions
Forced flow with axial velocity

a facing, parallel, porous, non-rotating surface

a solid rotating surface of infinite extent in the *r*, θ plane

Equation systems

- **Conservation equations**

Mixture continuity:

$$\frac{1}{\rho}\frac{\partial \rho}{\partial t} = -\frac{\partial u}{\partial x} - 2V - \frac{u}{\rho}\frac{\partial \rho}{\partial x} = 0 \qquad (1)$$

Radial momentum:

$$\rho\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(\mu\frac{\partial V}{\partial x}\right) - \rho\mu\frac{\partial V}{\partial x} - \rho\left(V^2 - W^2\right) - \frac{1}{r}\frac{dp_m}{dr} = 0 \qquad (2)$$

Circumferential momentum:

$$\rho\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(\mu\frac{\partial W}{\partial x}\right) - \rho\mu\frac{\partial W}{\partial x} - 2\rho VW = 0 \qquad (3)$$

Viscosity parameters

- **Viscosity of Gas mixture**

Viscosity of each gas species is defined by:

$$\mu_i = \frac{2.6693\times 10^{-5}\sqrt{M_i T}}{\sigma_i^2 \Omega_{\mu_i}} \xrightarrow{\text{rewritten as}} \mu_i = \delta_{1i} T^{\psi_{1i}}$$

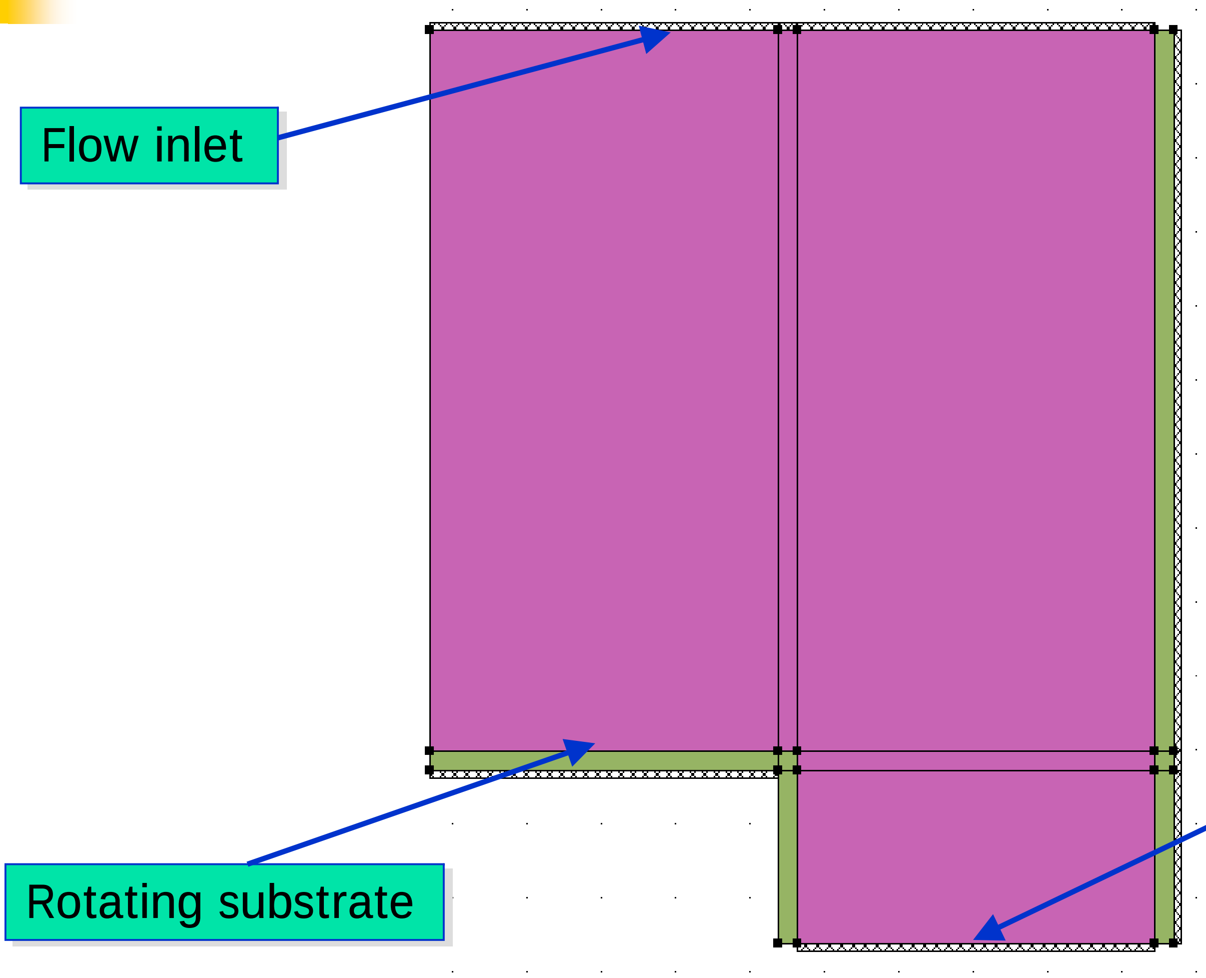
Viscosity of gas mixture is calculated with the Wilkes correlation:

$$\mu_{mix} = \sum_{i=1}^{n} \left(x_i \mu_i \middle/ \sum_{j=1}^{n} x_i \Phi_{ij} \right)$$

$$\Phi_{ij} = \left[1 + \left(\mu_i / \mu_j\right)^{1/2} \left(M_i / M_j\right)^{1/4}\right]^2 \Big/ \left[8 + 8\, M_i / M_j\right]^{1/2}$$

Example of GaN growth in vertical reactor with Rotating-Disk

Structure

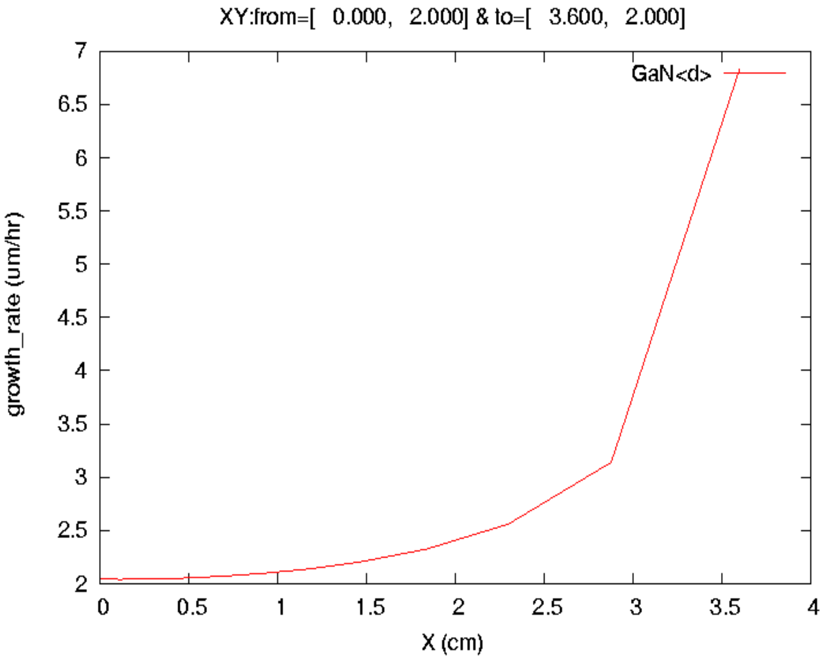

Flow inlet

Flow outlet

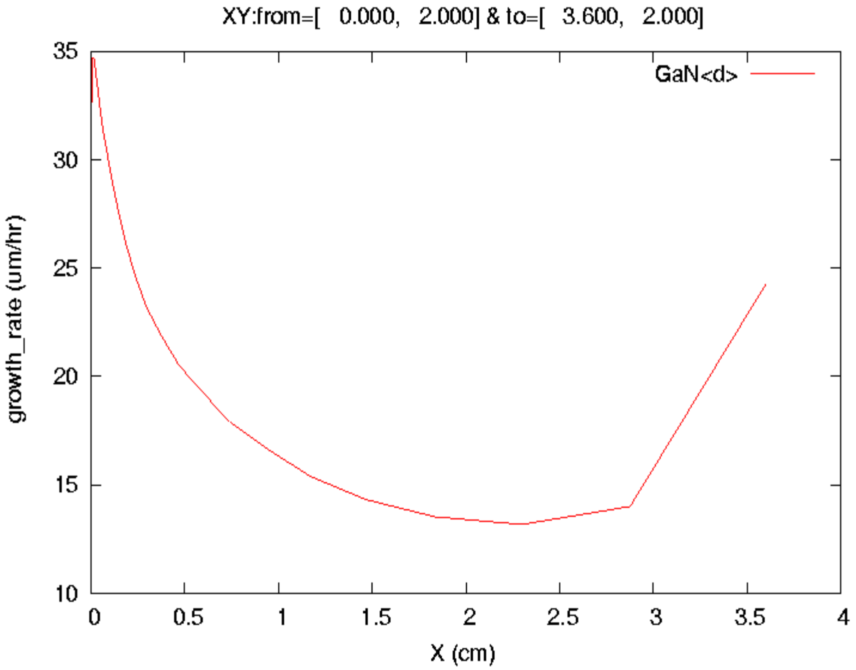
Rotating substrate

Vertical reactor described by cylindrical coordinate

Effects of rotating disk



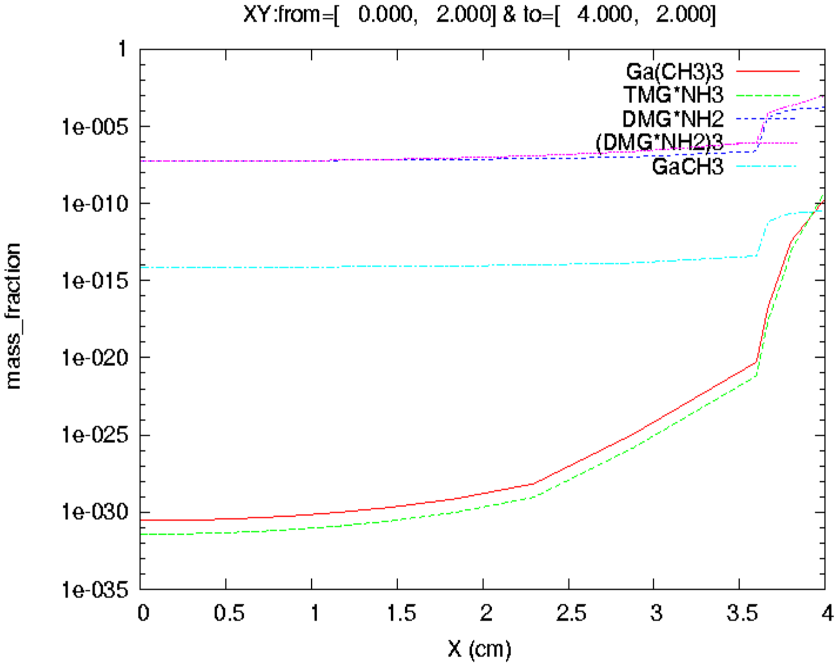
Rotating rate=0 rpm

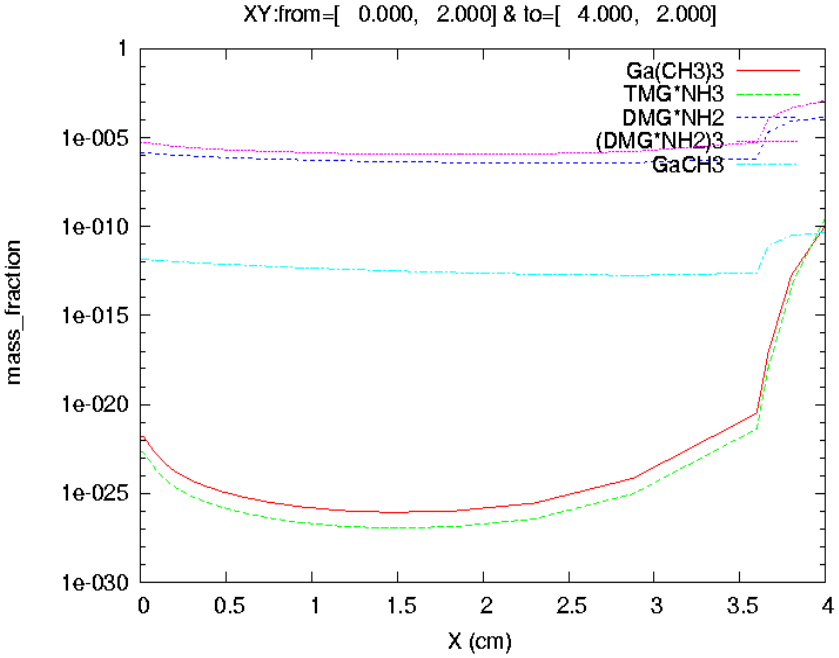


Rotating rate=1000 rpm

Rotating disk increases GaN growth rate especially near the center of the substrate

Performace Compared



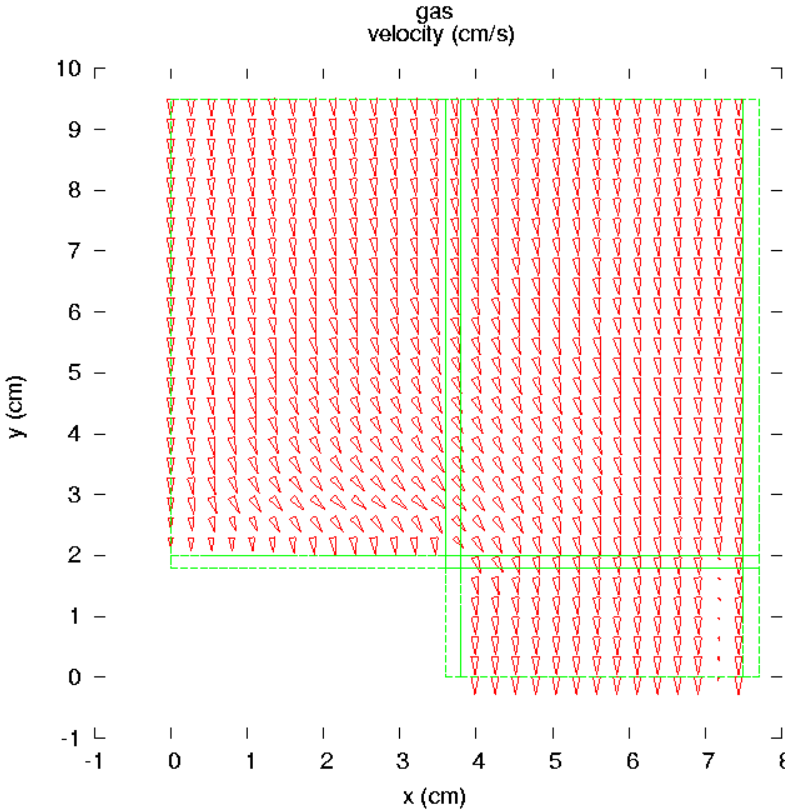


Rotating rate=0 rpm

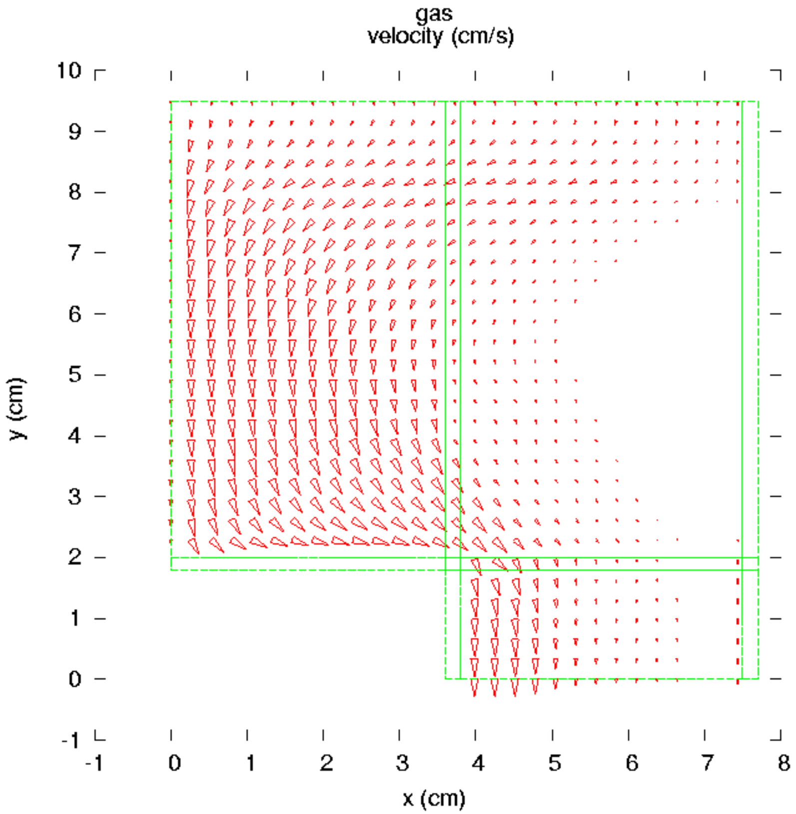
Rotating rate=1000 rpm

More mass fraction of species tend to concentrate at center for rotating disk

Performace Compared



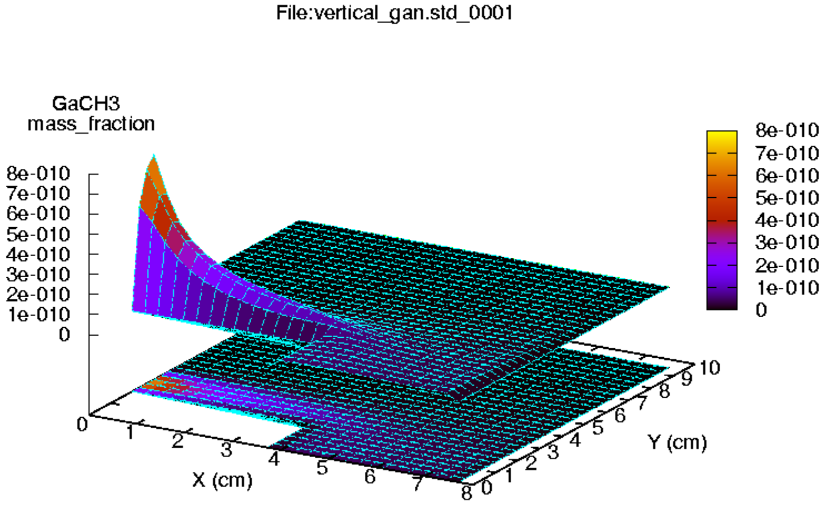
Rotating rate=0 rpm



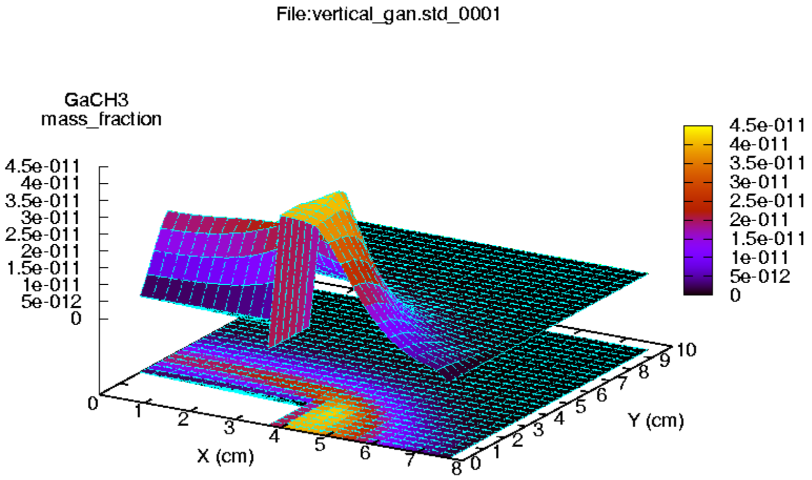
Rotating rate=1000 rpm

The rotating disk attracts the flow towards disk center.

Performace Compared



Rotating rate=1000 rpm

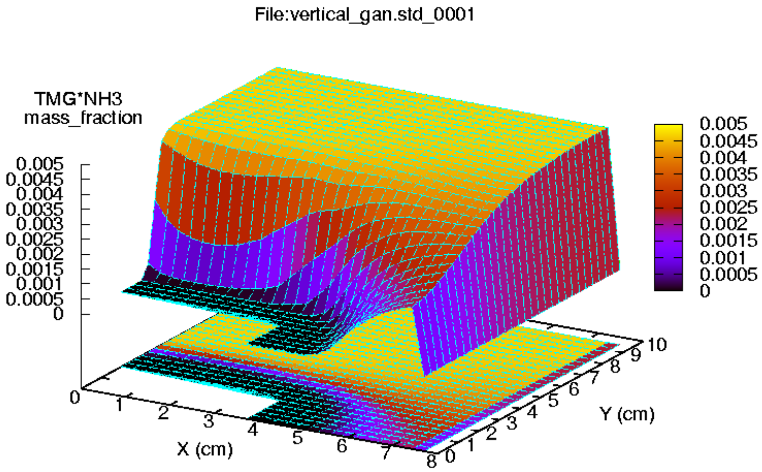


Rotating rate=0 rpm

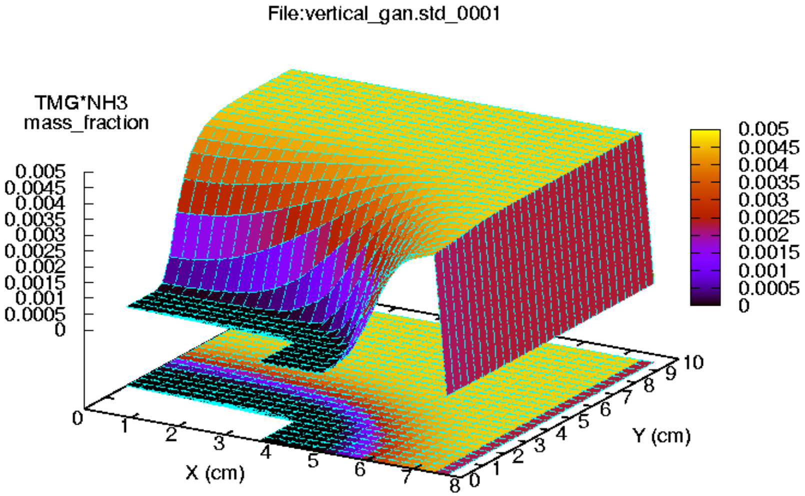
Most of GaCH3 gathers and takes part in the chemical reaction in the region of a rotating substrate.

Nevertheless, lots of it flow out from the outlet with a immobile substrate.

Performace Compared



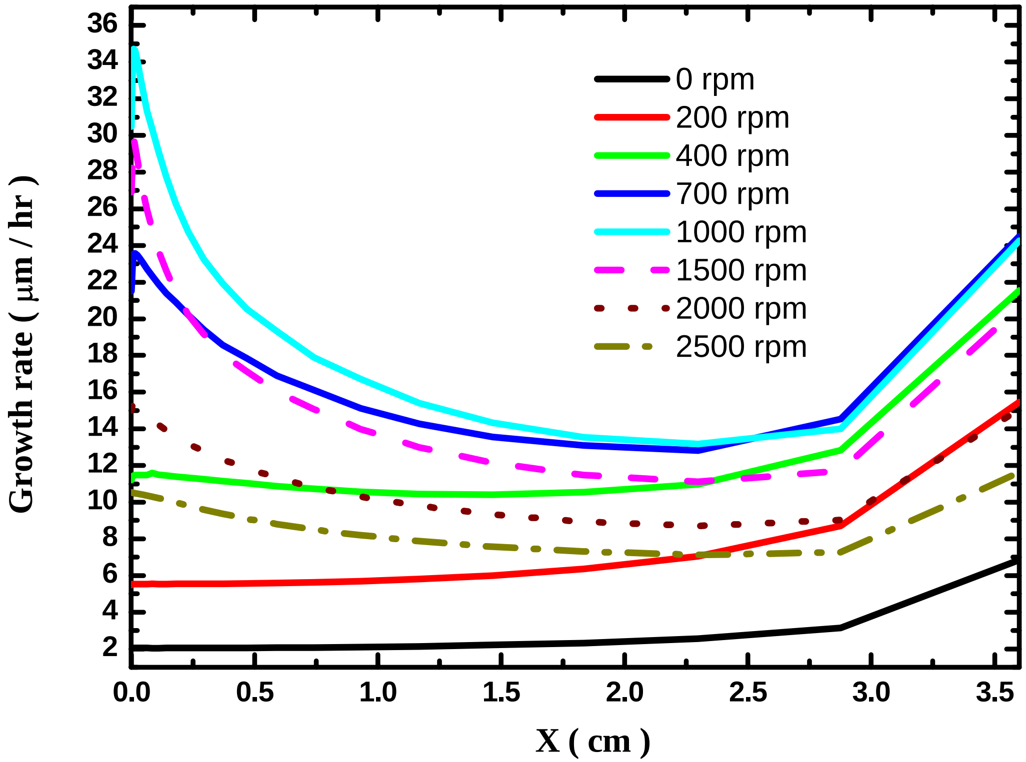
Rotating rate=1000 rpm



Rotating rate=0 rpm

More TMG*NH3 flows to the region of substrate under the rotation than that without the effect, which is beneficial to the growth of GaN.

Performace Compared



Remark: At lower RPM, rotation increases growth rates of GaN by attracting species to the disk center. At higher RPM, larger radial velocity leads to more species leaking towards the outlet without having a chance to be deposited on substrate.

Pressure_gradient_const=0.01, RPM_ref=1500 rpm

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Summary

- PROCOM offers a comprehensive model of MOCVD process taking into account fluid dynamics, mass and heat transports, and non-equilibrium gas-gas, gas-surface chemical reactions.
- Rather comprehensive GUI tools are developed to handle geometry, mesh and chemical reaction design controls.
- The rotating disk model is efficient and clearly demonstrates the benefits of using a rotating disk in MOCVD.