Reactor Design Optimization Based on 3D CFD Modeling of Nitrides Deposition in MOCVD Vertical Rotating Disc Reactors

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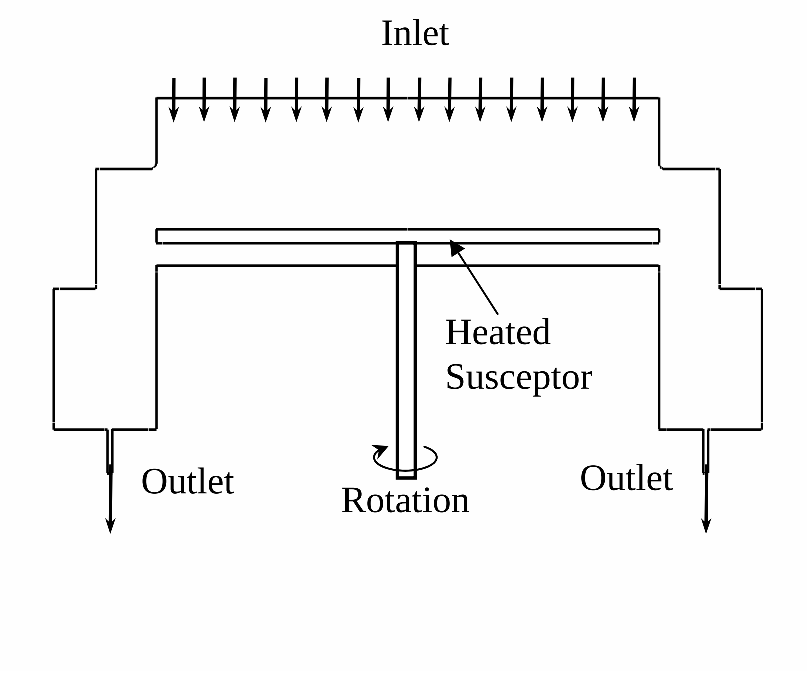
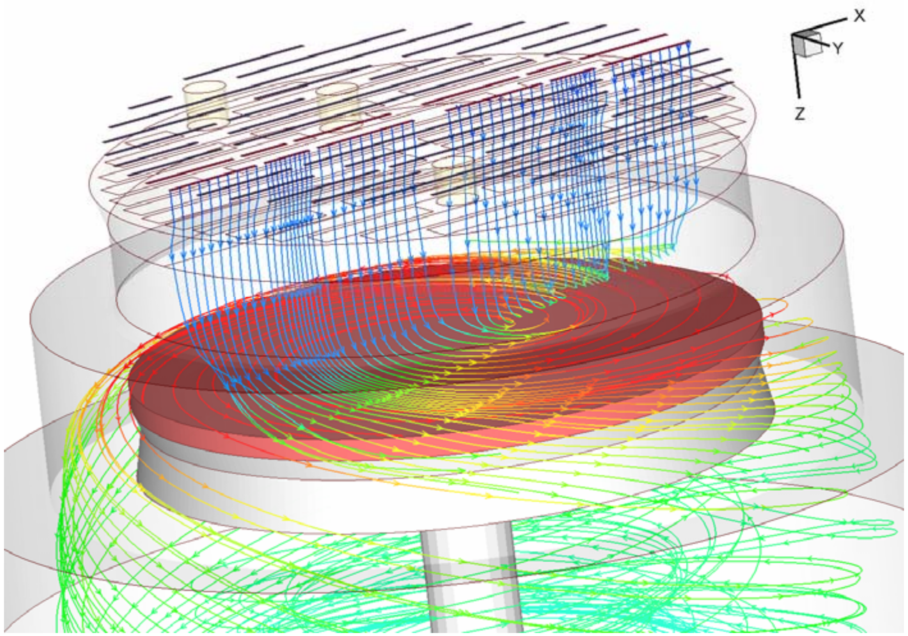
Introduction

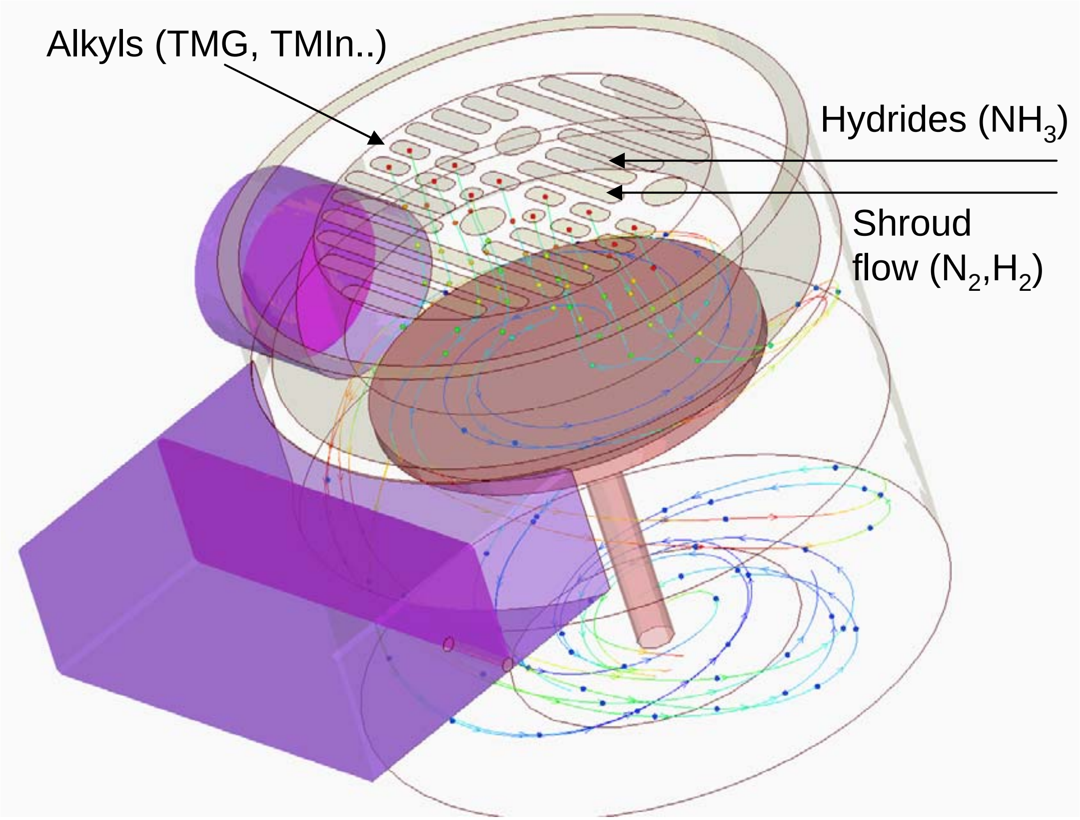
- MOCVD (Metal-Organic Chemical Vapor Deposition) Vertical Rotating Disc Reactors (RDR) are widely used for the large-scale production of GaN-based semiconductor devices such as blue and green light-emitting diodes (LED), ultra violet LED, solid-state lasers, heterojunction bipolar transistors.
- In RDRs rotation of the wafer carrier results in an effective averaging of the deposition rate distribution and this is a key mechanism providing growth of epitaxial layers with highly uniform properties.





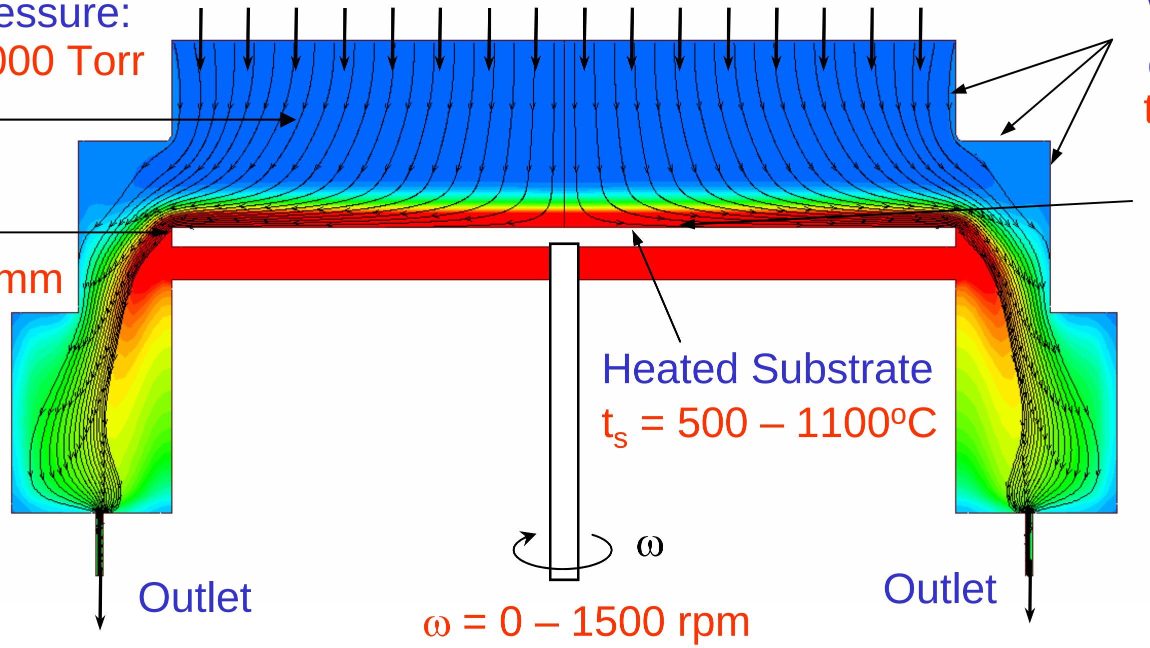
Introduction

- The necessity to utilize a number of different precursors for nitride deposition, many of which actively react with each other in the gas phase, presents significant challenges for the reactor development, particularly the reactant injection elements.



- Proper design of such components is practically impossible without detailed flow modeling based on CFD that addresses optimization of both reactor components and process parameters and is based on an ability to predict GaN/InGaN growth rate and uniformity under different process conditions.

Geometry and Process Parameters in the Veeco MOCVD TurboDisc Reactors



Inlet Gases (Reactants)
- Alkyls ($Ga(CH3)_3$, $In(CH3)_3$..)
- Hydrides (NH_3)
- Shroud flow (N_2,H_2)

Total Flow Rate:
Q = 5 – 250 slm

Reactor Pressure:
P = 50 – 1000 Torr

Water-cooled walls
t_w = 25 – 75°C

Diameter
d = 75 – 450 mm

Solid Products:
GaN, InGaN, AlGaN …

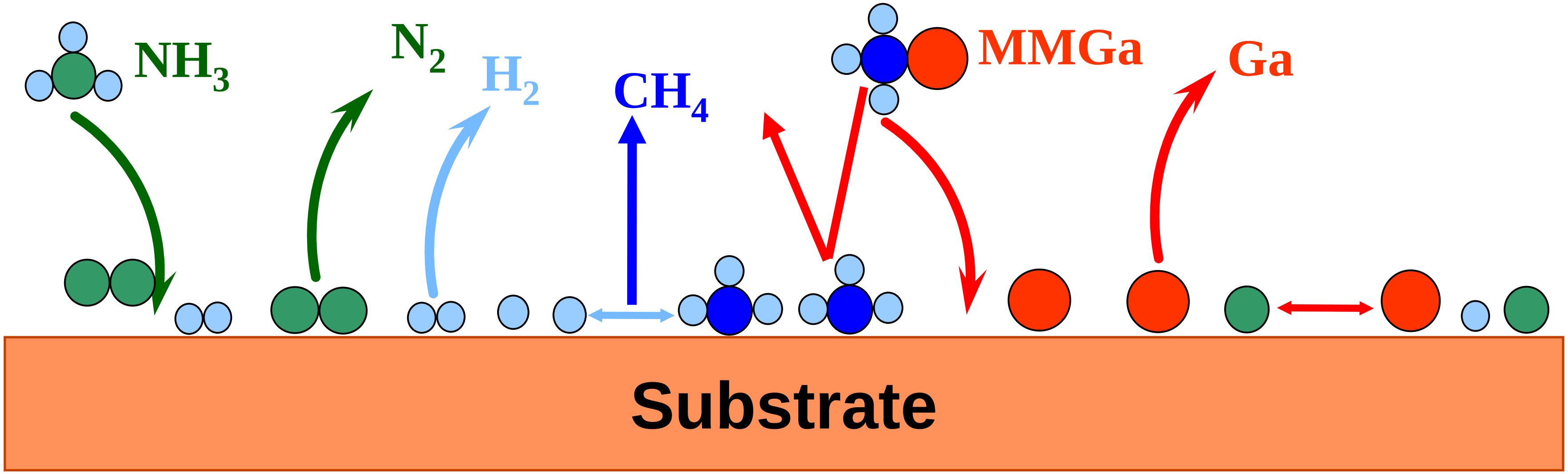
Heated Substrate
t_s = 500 – 1100°C

Outlet

Outlet

ω = 0 – 1500 rpm
Spindle

Surface chemical processes during GaN growth

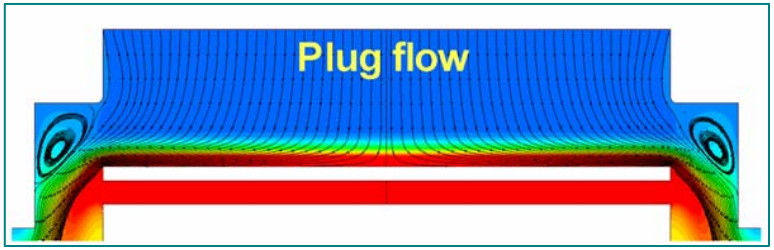


Rate-limiting processes

- *Low temperatures (400-600 ºC):* group-III adsorption site blocking by methyl radicals
- *Intermediate temperatures (600-1050 ºC):* transport of group-III species to the growth surface
- *High temperatures (above 1050 ºC):* gallium desorption

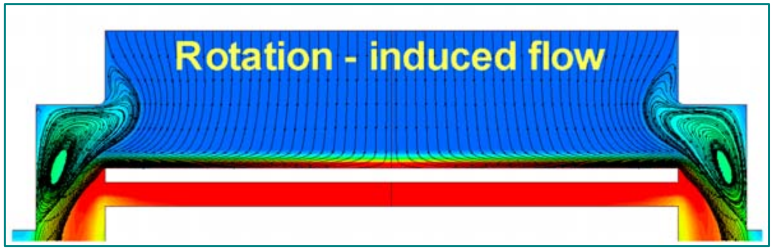
Flow Dynamics in Rotating Disc MOCVD Reactors

- Rotating Disc MOCVD Reactors involve complex flow dynamics driven by interactions between buoyancy forces, wafer carrier rotation and forced convection.

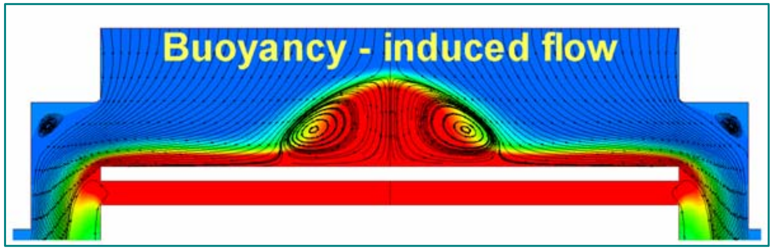


Gas flows smoothly over the substrate without any recirculations above the wafer carrier

- There is considerable interest in understanding and controlling reactor gas flow dynamics as the flow regimes in the process reactor are largely responsible for compositional and thickness non-uniformity.



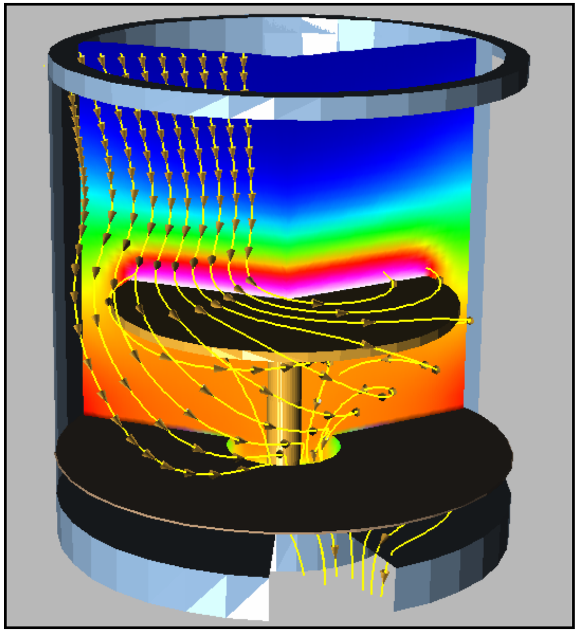
Vortex forms near the reactor wall close to the upper disc surface



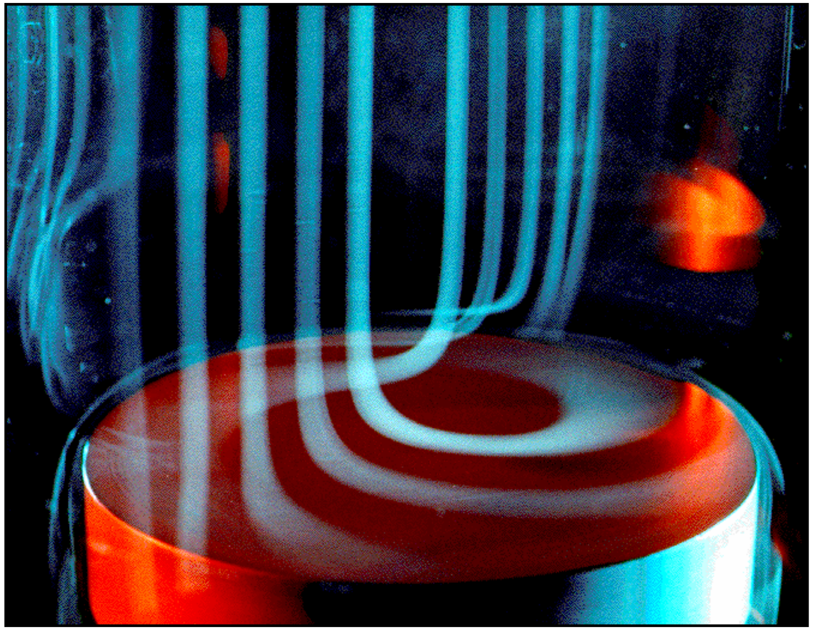
Thermal recirculation – density difference between the disk and the incoming gas stream overcomes the stabilizing influence of the viscous forces

Flow Patterns in the Rotating Disc Reactors

Computer Generated Flow Patterns in Rotating Disc System



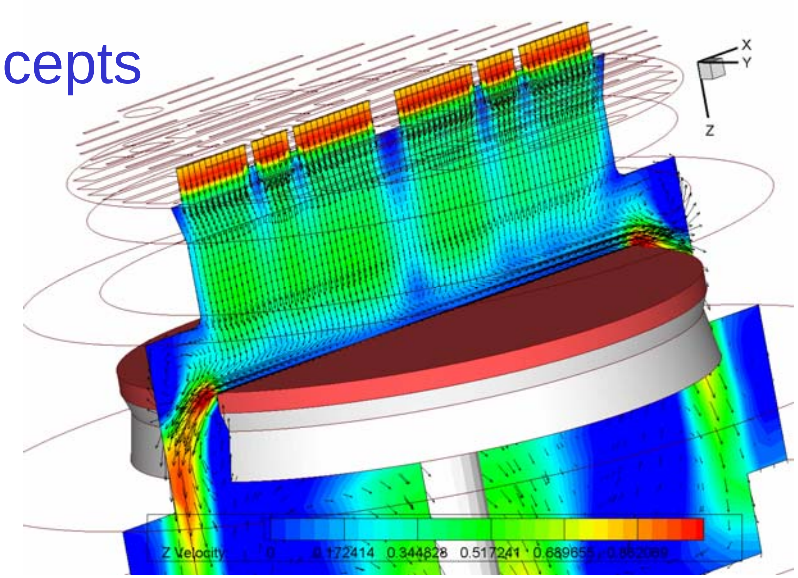
Smoke Flow Patterns in Rotating Disc System



Data Courtesy of Sandia National Laboratories

CFD Modeling at Veeco TurboDisc Operations

Reactor and process development guided by CFD

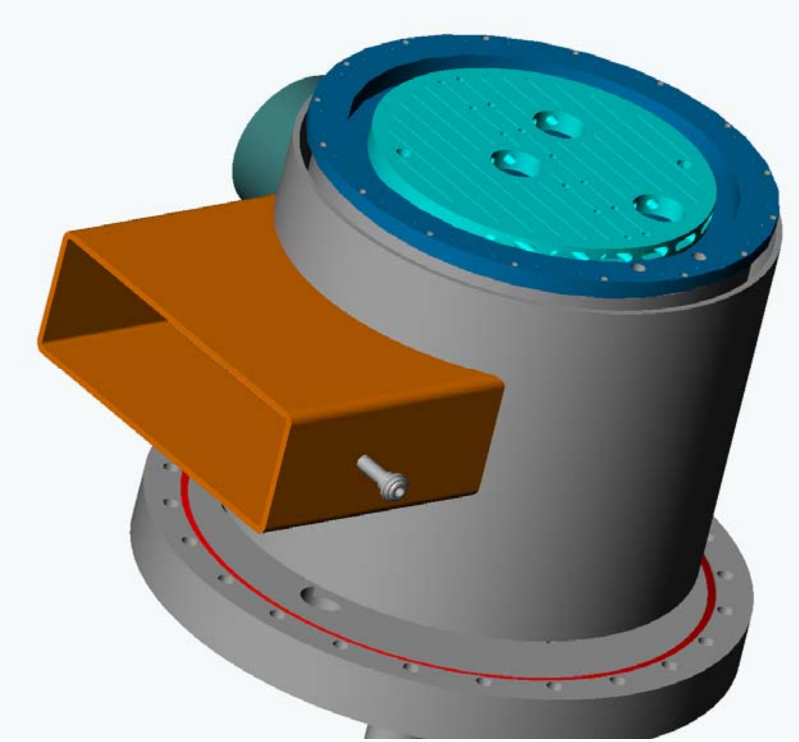


- Feasibility, evaluation of design concepts
- Equipment design optimization
- Process optimization
- Customer support

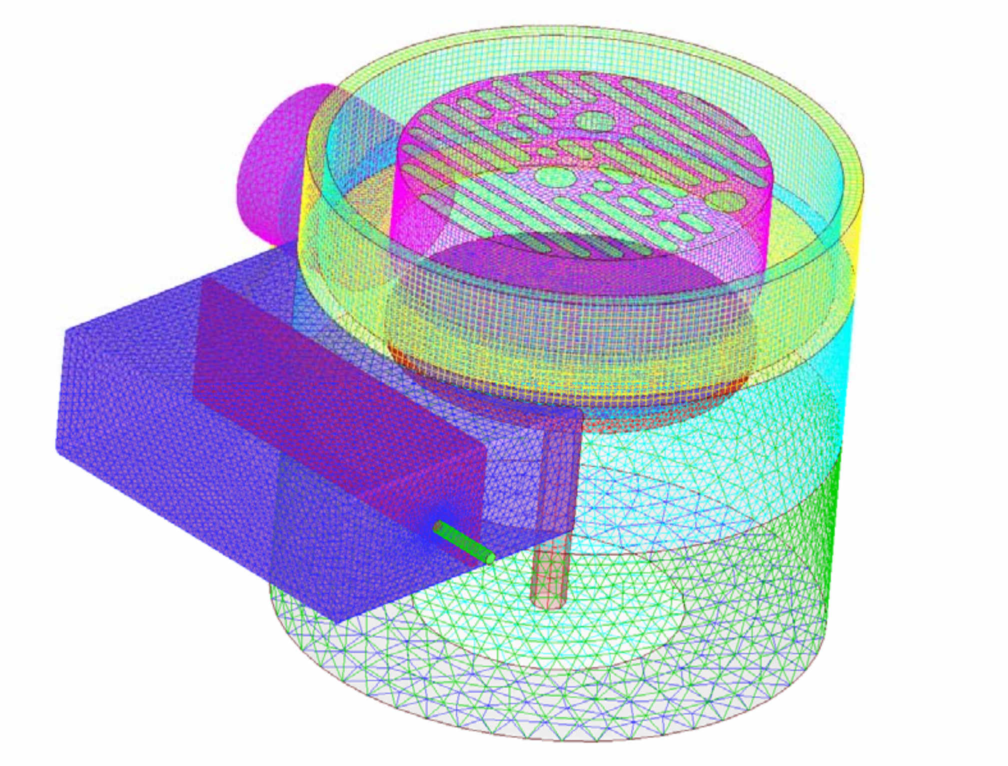
- Commercial CFD solver FLUENT by Fluent Inc.
  flow dynamics, heat and mass transport of precursors and reaction products, chemical reactions.

Solid Works Example – D125GaN Reactor

model

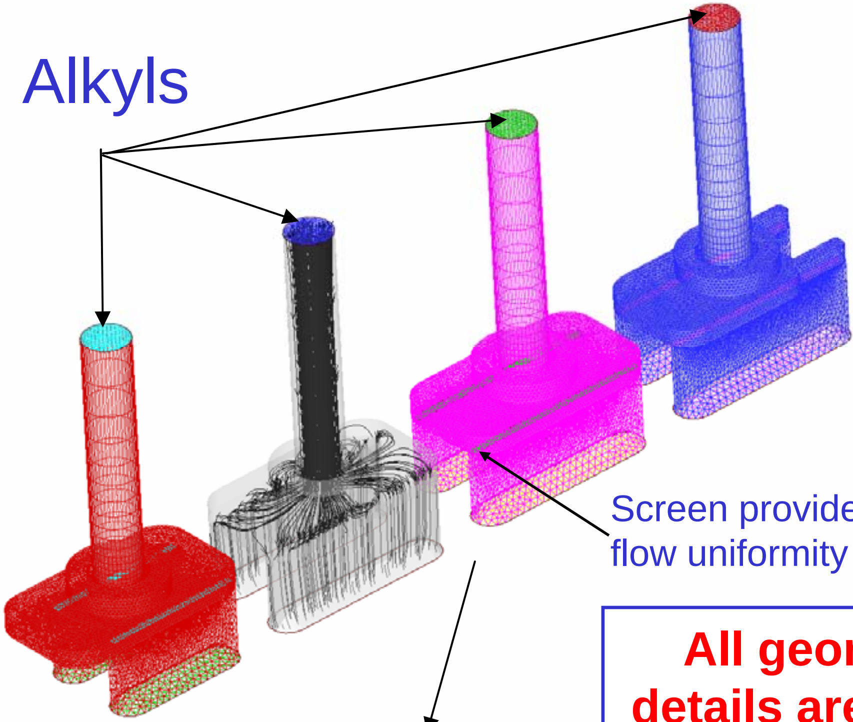


mesh



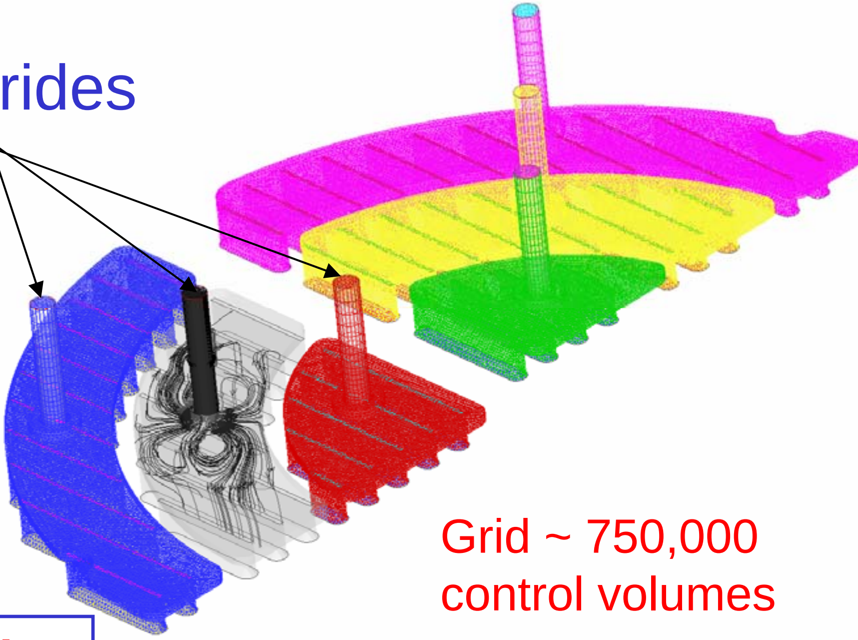
Solid Works (Computer Aided Design Software) models are used for the grid generation by direct import to CFD code

Alkyls



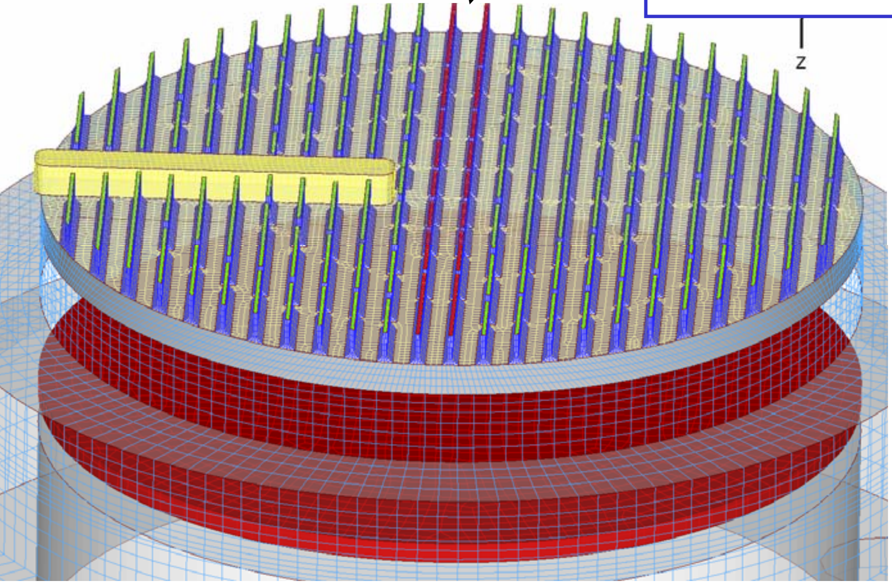
Screen provides flow uniformity

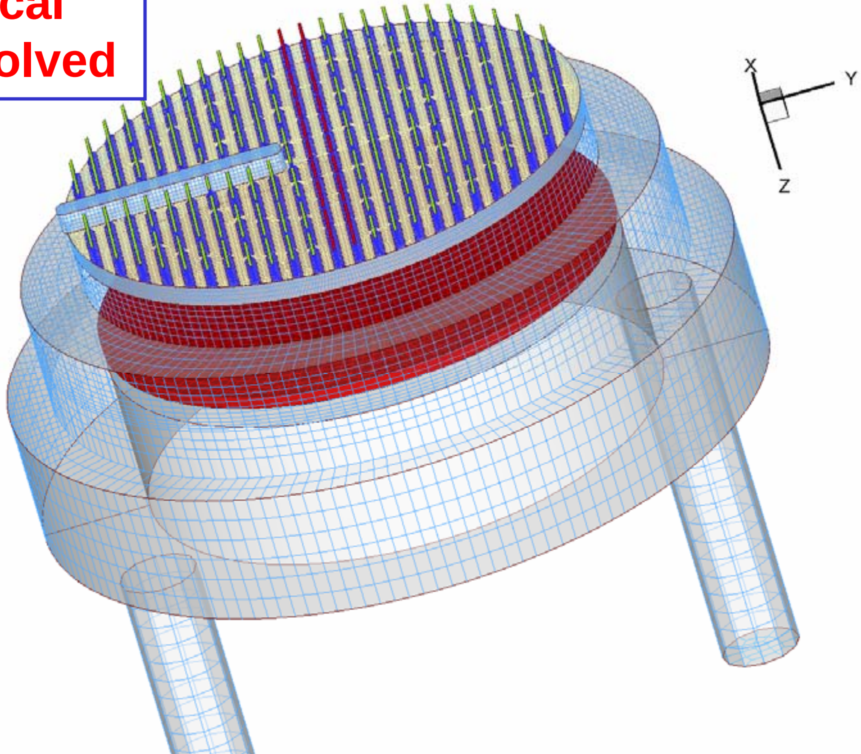
Hydrides



Grid ~ 750,000 control volumes

All geometrical details are resolved

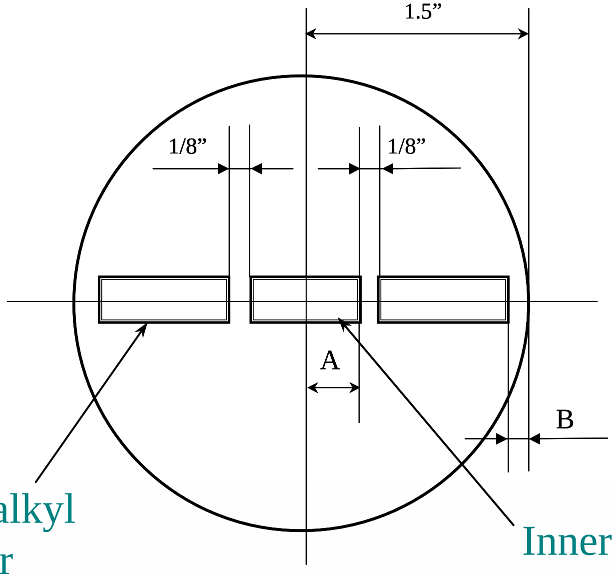




CFD – DOE Optimization of the Injector Plate

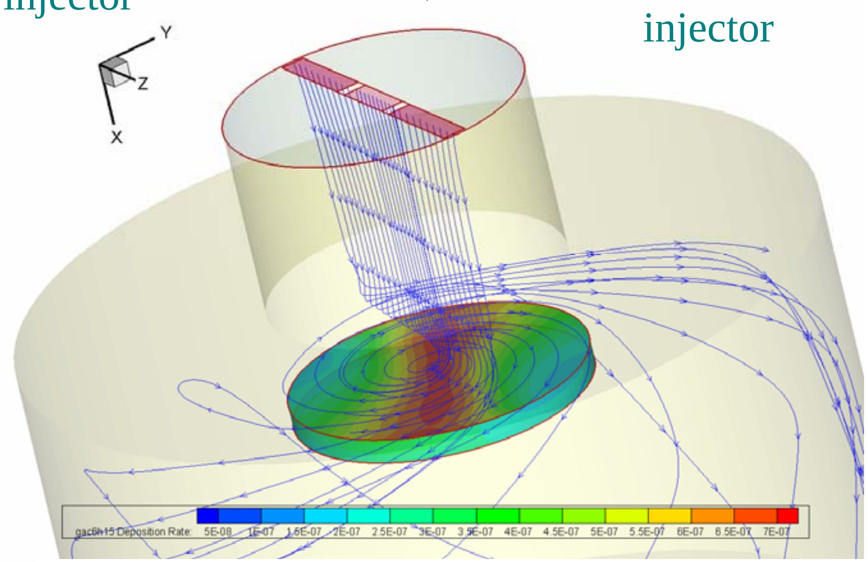
Objective:

Find the optimal sizes and positions of the alkyl zones (parameters A and B) that provide the best growth rate deposition uniformity on the wafer in a wide range of process conditions

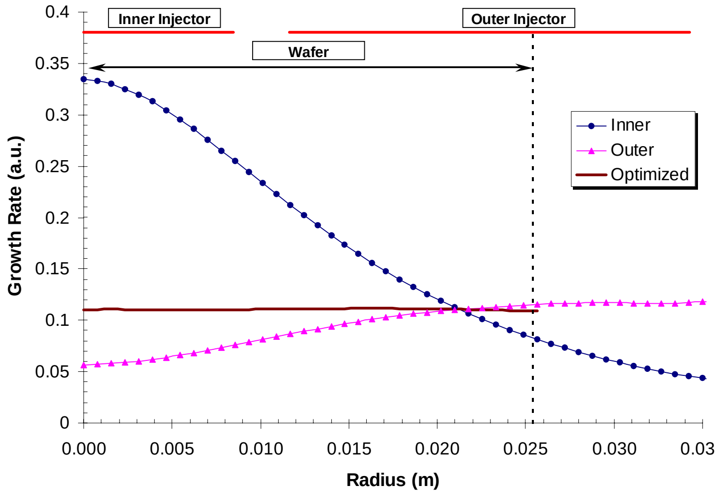


Outer alkyl injector

Inner alkyl injector

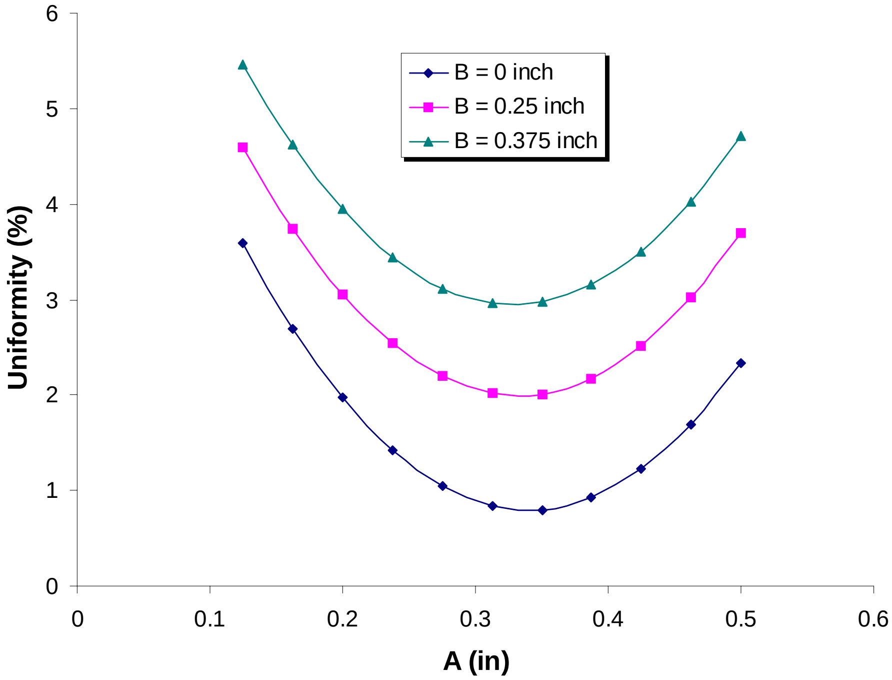


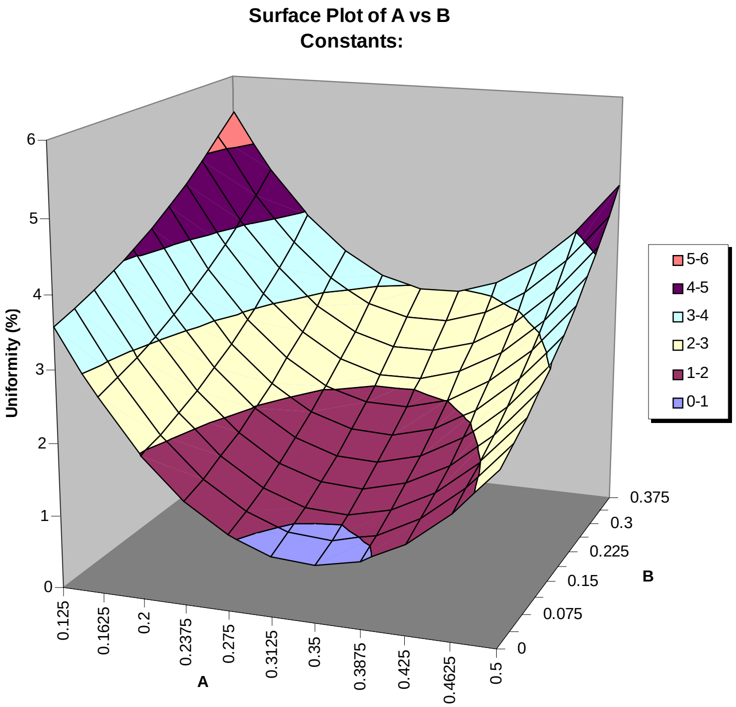
Simplified model – streamlines and growth rate



Superposition technique (L.Kadinski et al., Jounal of Crystal Growth 261, 2004., 175-181)

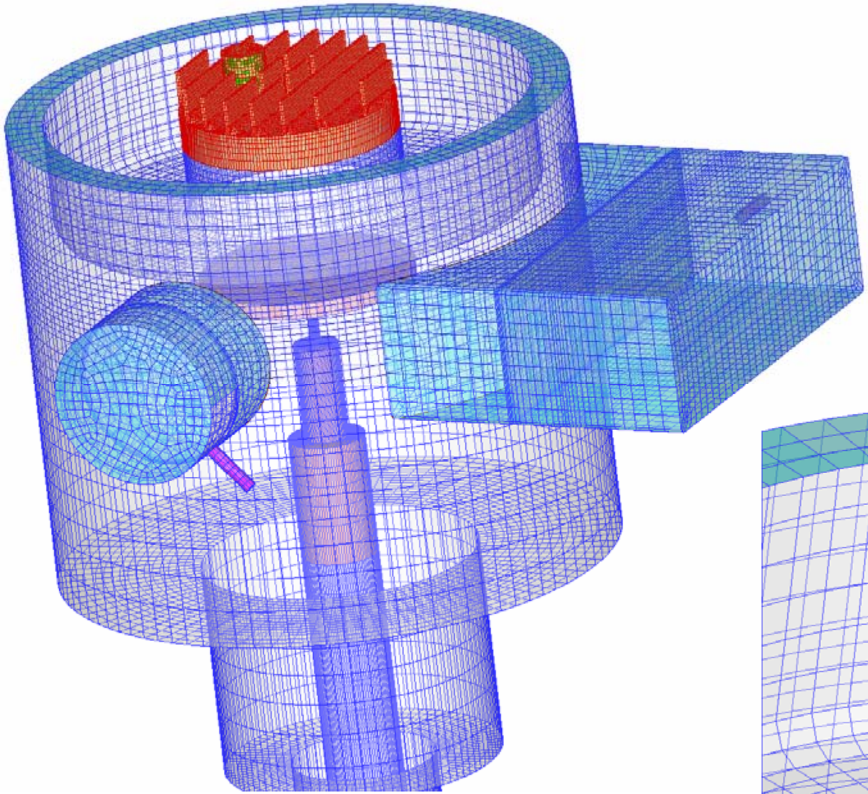
CFD – DOE Optimization of the Injector Plate



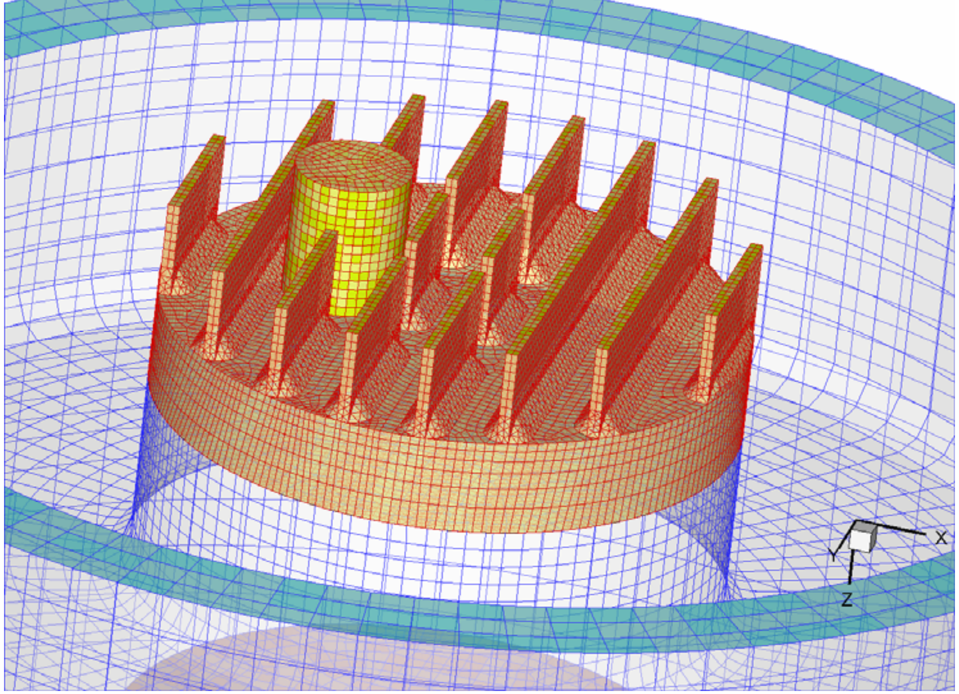


An optimal geometrical position of the alkyls zones is found for different process conditions which correspond to GaN based LED process development

Detailed numerical grid of P75 VEECO Reactor and of Flow Flange

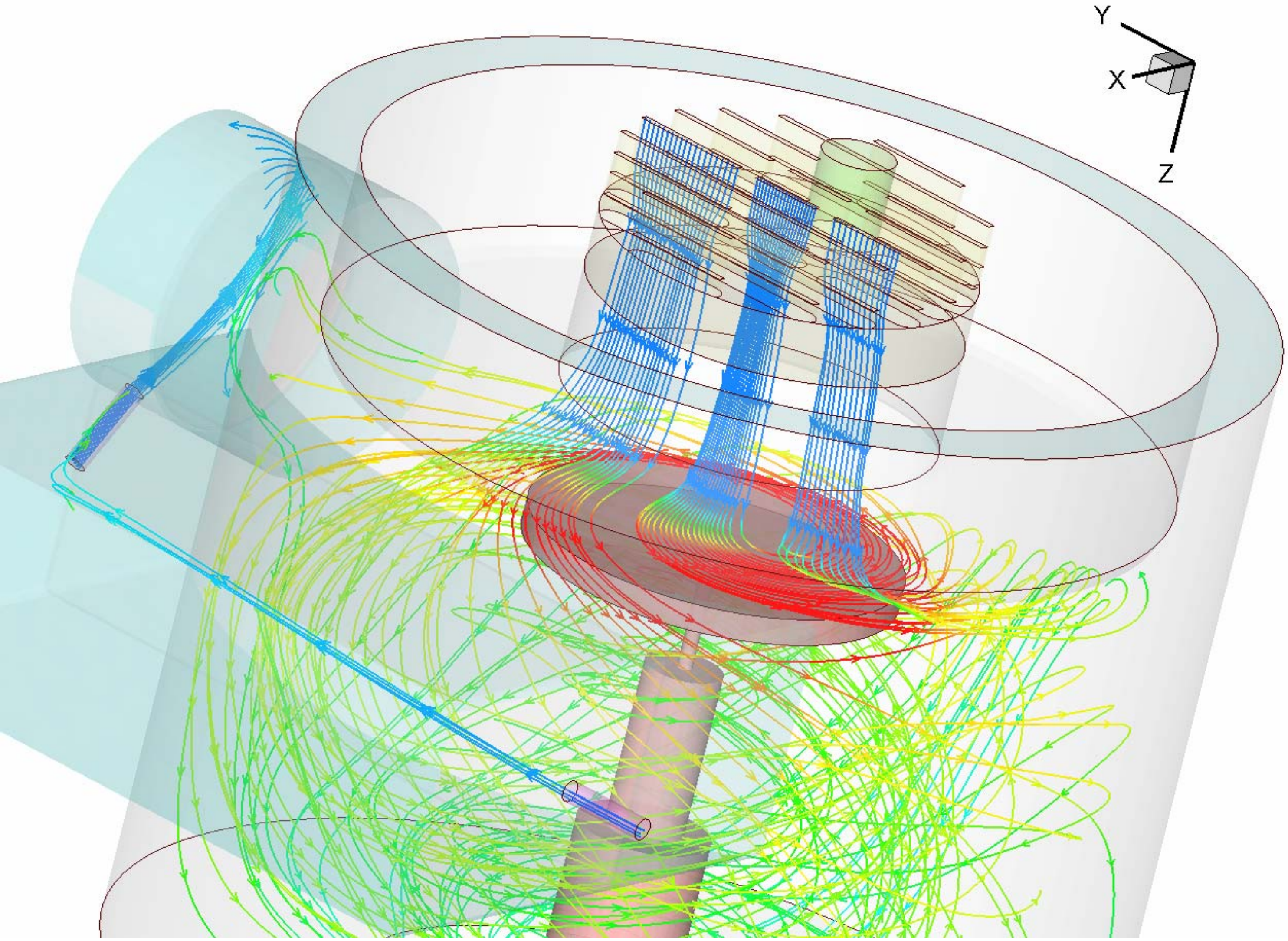


Grid: 500,000 control volumes



Based on the optimized injector plate a new modification of P75 TurboDisc Reactor has been designed

Flow Visualization in the P75 Reactor

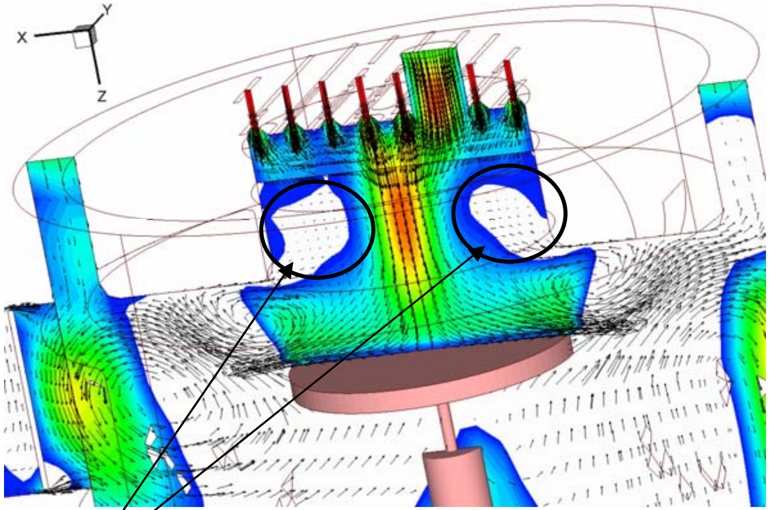


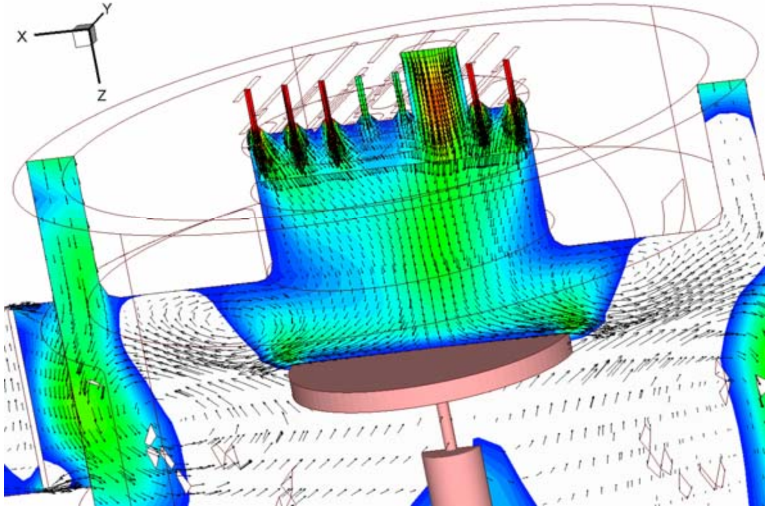
Flow Optimization in the Reactor

Velocity matched conditions between alkyl and hydride zones

Velocity profiles

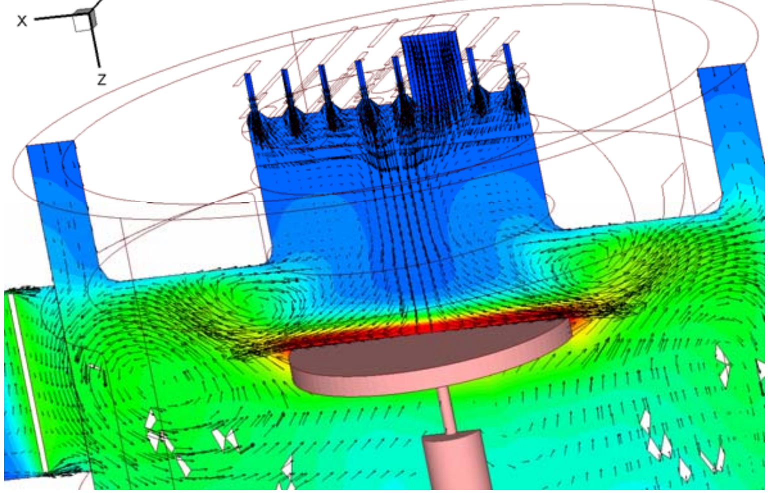
Momentum matched conditions between alkyl and hydride zones

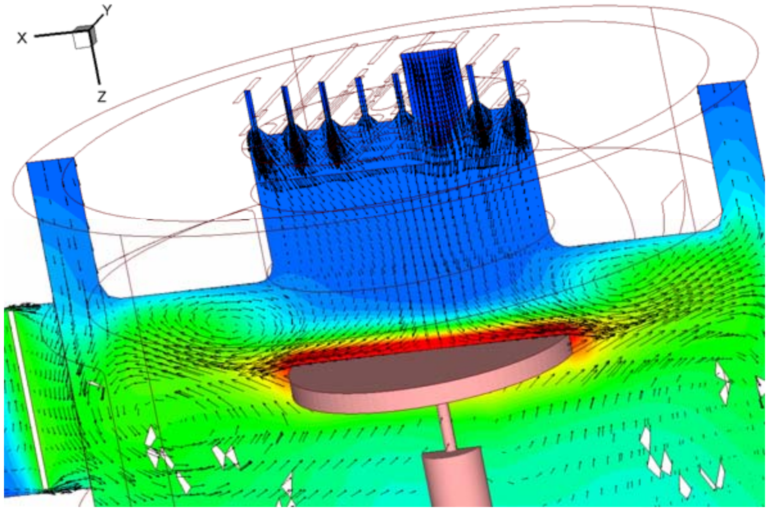




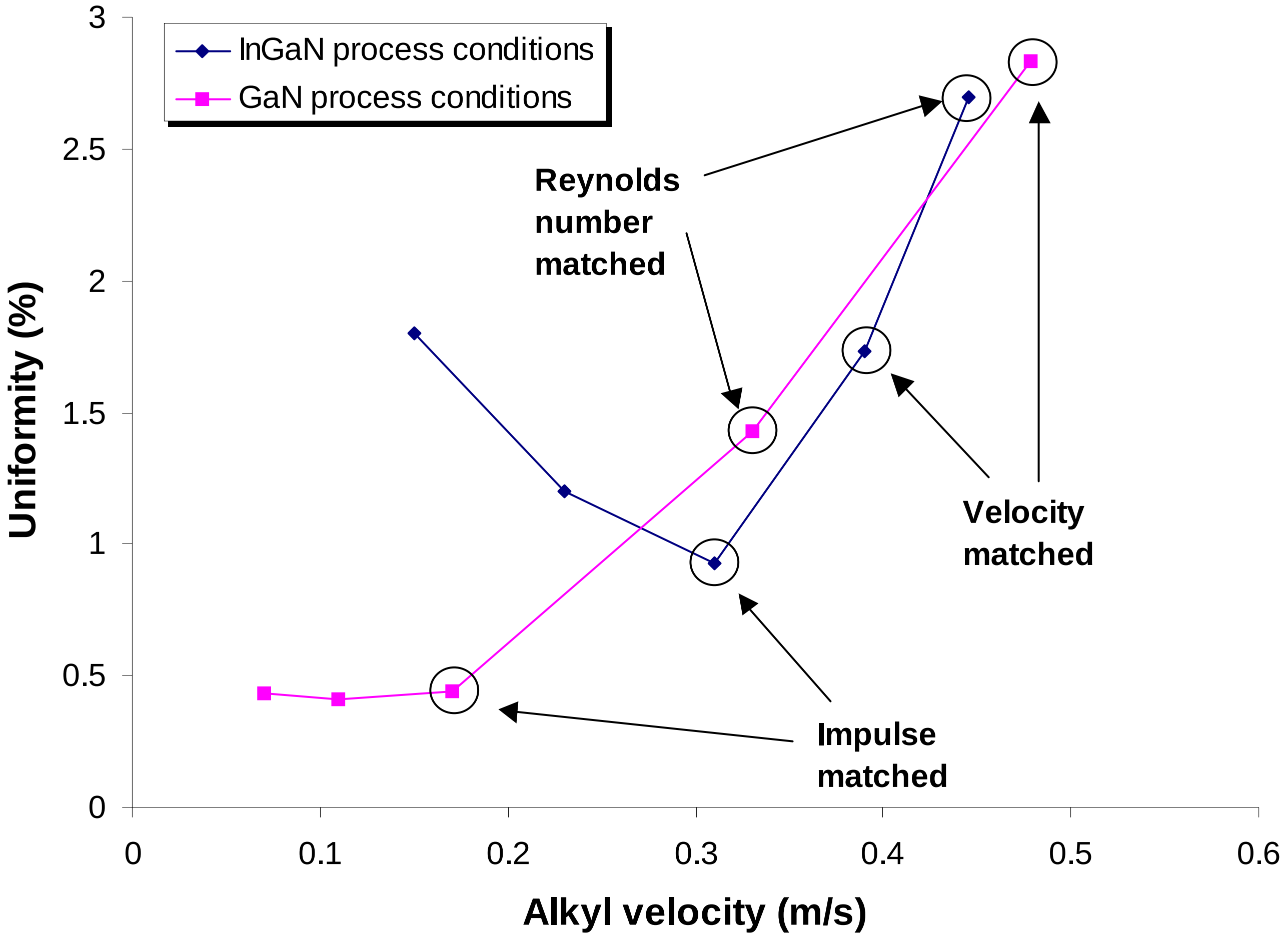
Recirculation areas

Temperature profiles



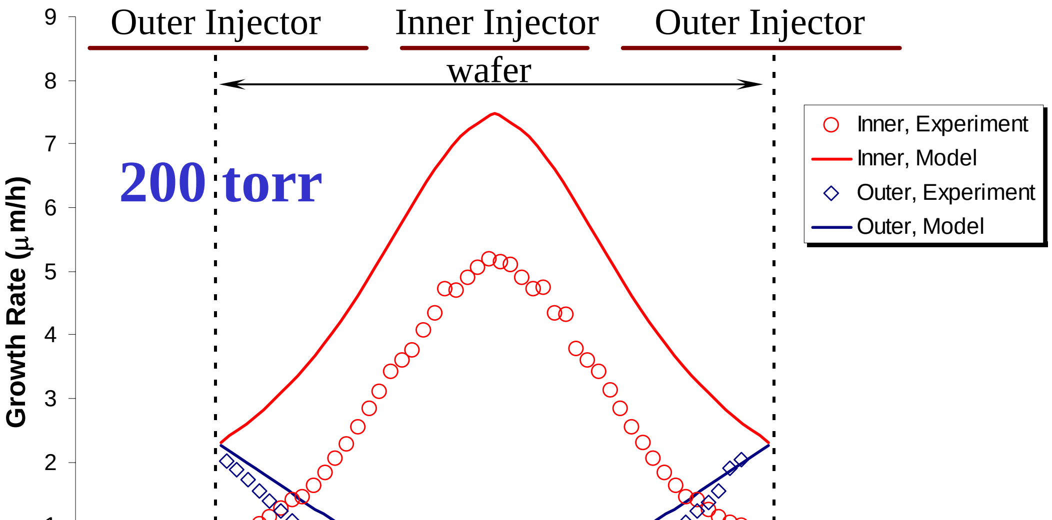


Flow Optimization in the Reactor



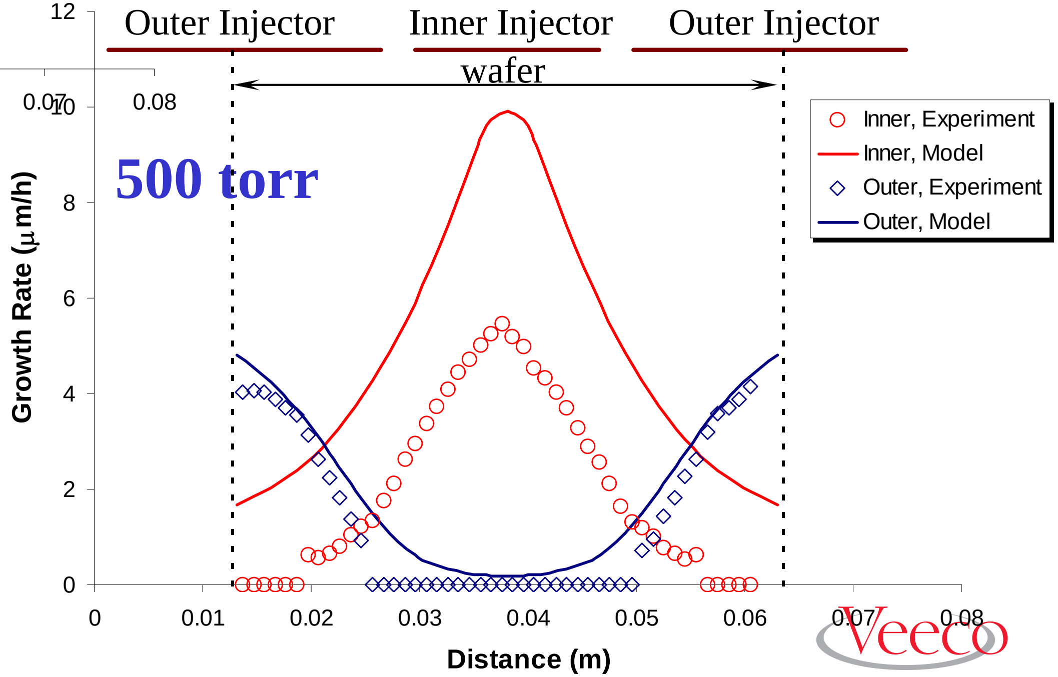
Impulse matched conditions provide flow with no recirculation and the best growth rate uniformity in P75 reactor

Experimental Verification - *Effect of Pressure*



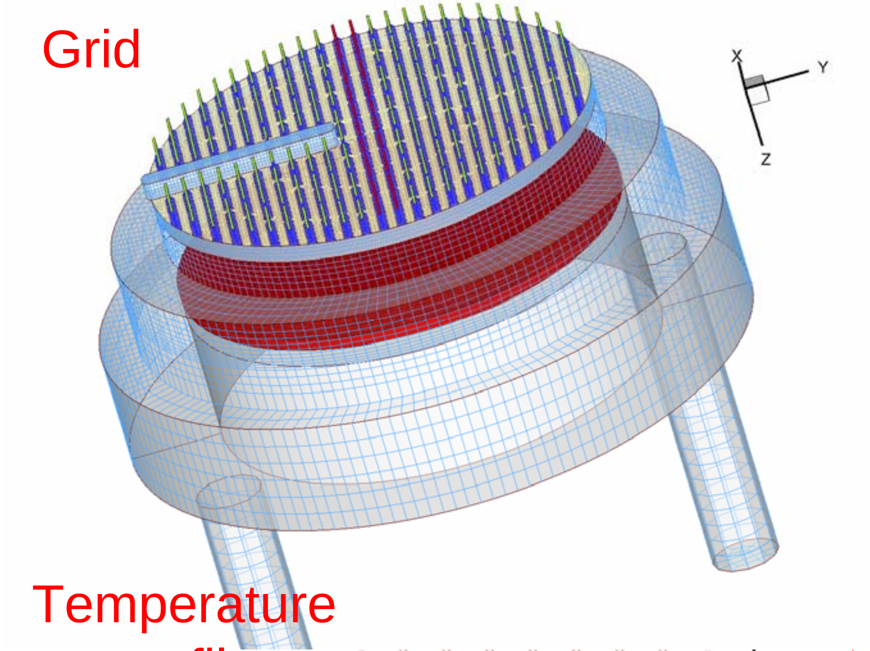
For superposition, a set of independent runs (a number of runs is equal to the number of alkyls zones) are conducted wherein each run, the alkyls flow into the reactor only in a single zone. All of the other zones contain push gas. Each run gives an individual growth rate/composition “response” for the zones

Excellent qualitative and solid quantitative agreement between the modeling results and experiments is observed

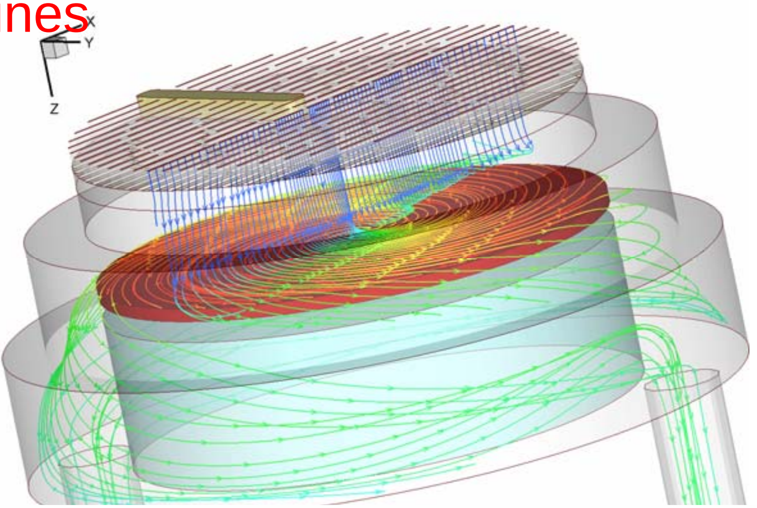


CFD Model for high capacity multi-wafer reactors

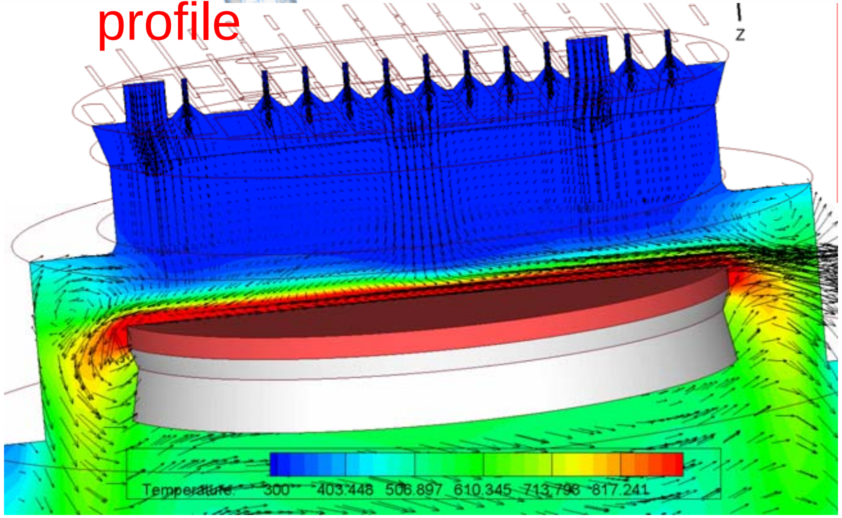
Grid



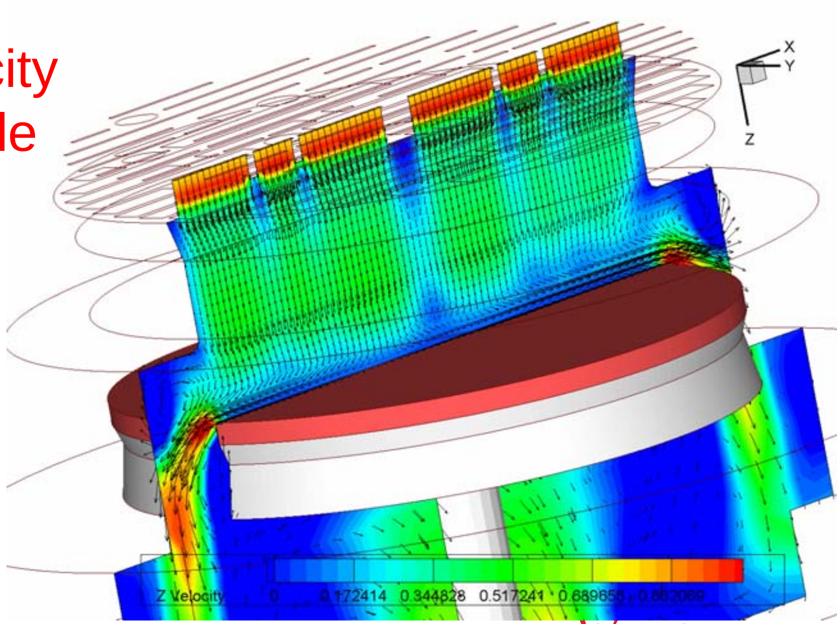
Streamlines



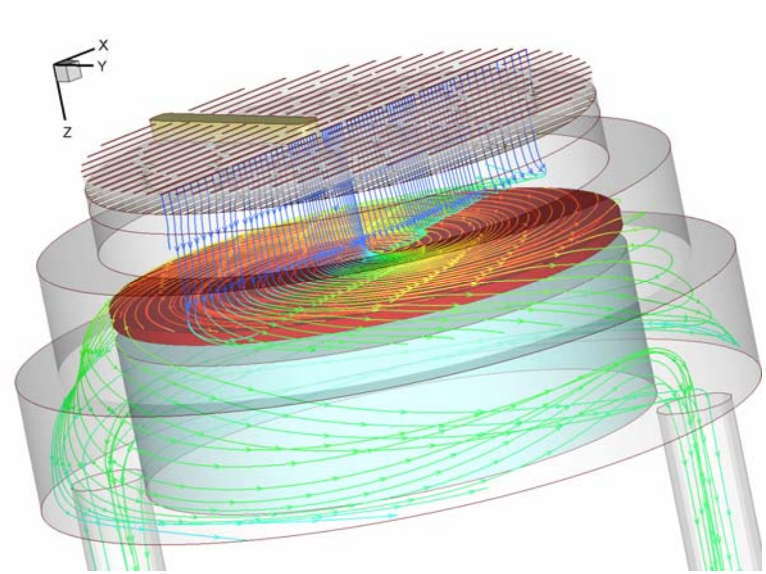
Temperature profile



Velocity profile



Comparison with the Experimental Data



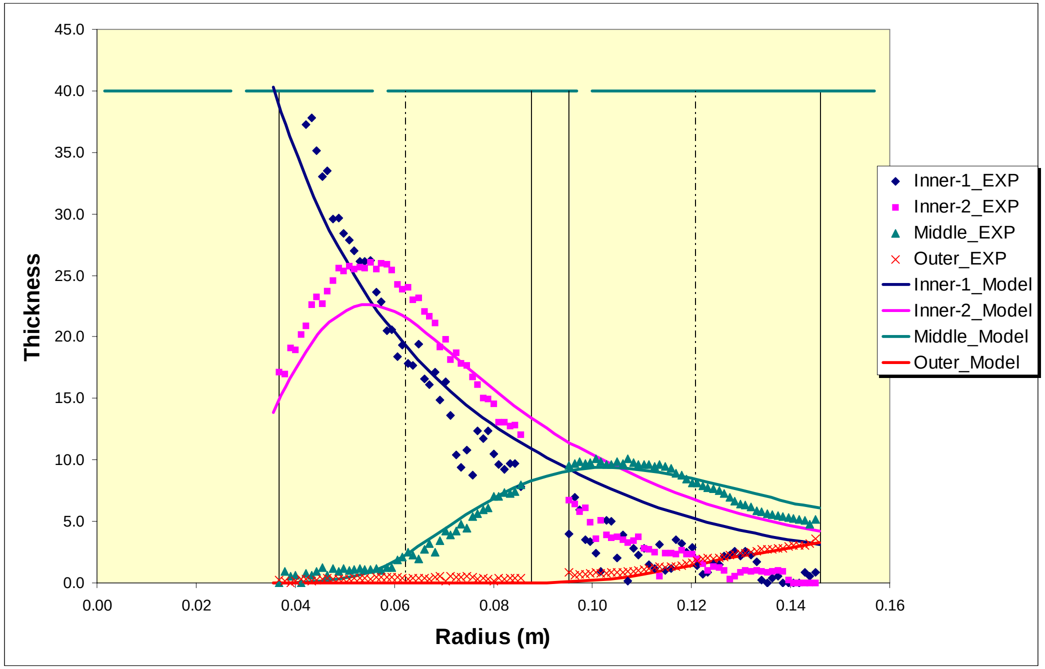
Good qualitative and quantitative agreement between the modeling results and experiments is observed

GaN Growth Conditions

P = 200 Torr **Q_{N2} = 15 slm**

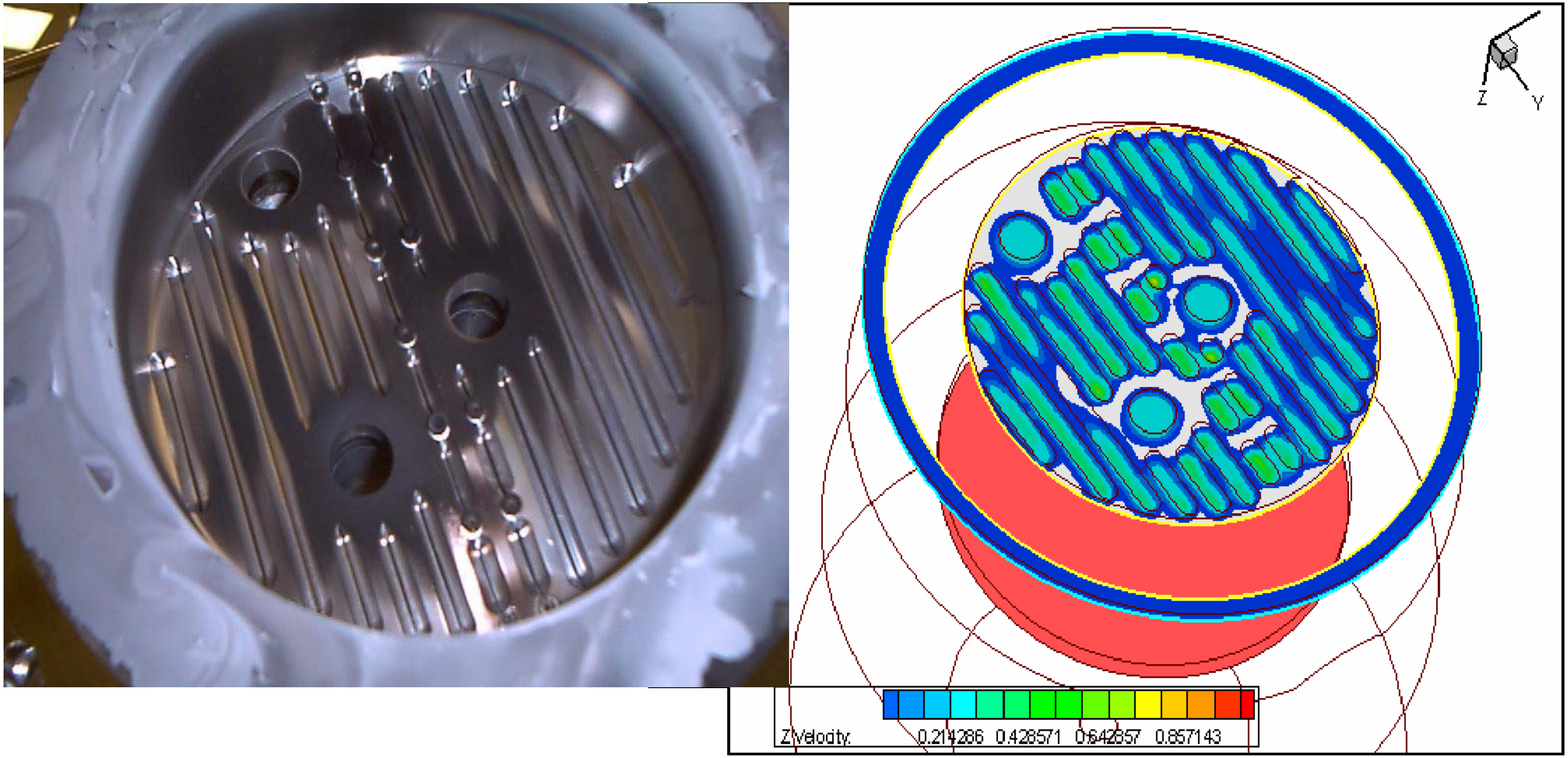
ω = 1500 rpm **Q_{H2} = 80 slm**

t_s = 1050 ^{o}C **Q_{NH3} = 40 slm**



Model Verification

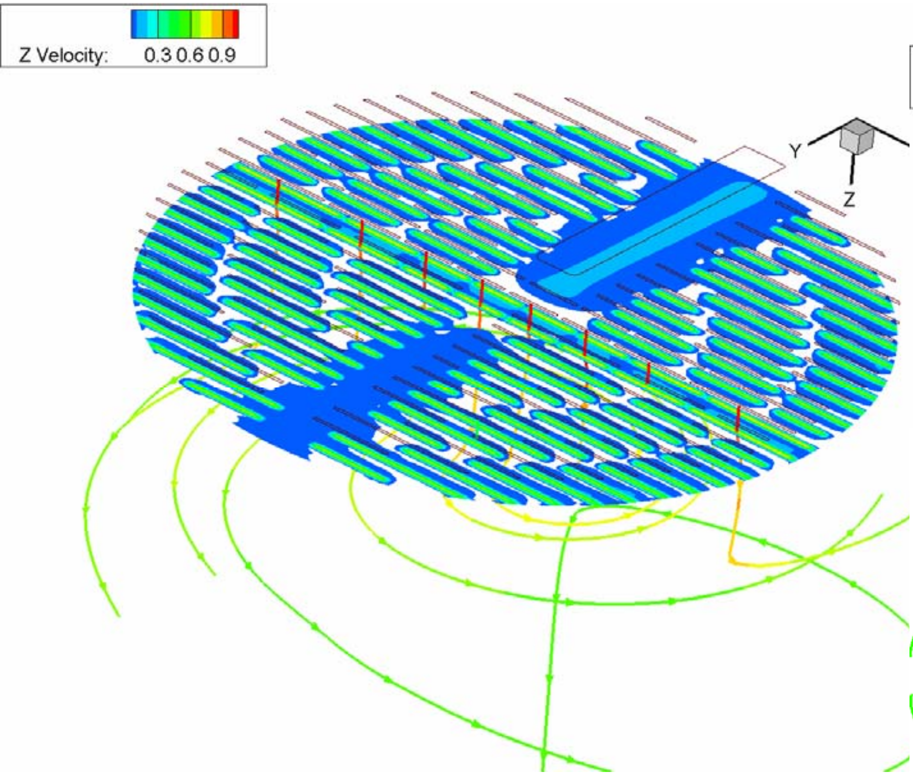
Developed CFD model helped us to identify the potential problems for the flow flange design of the reactor



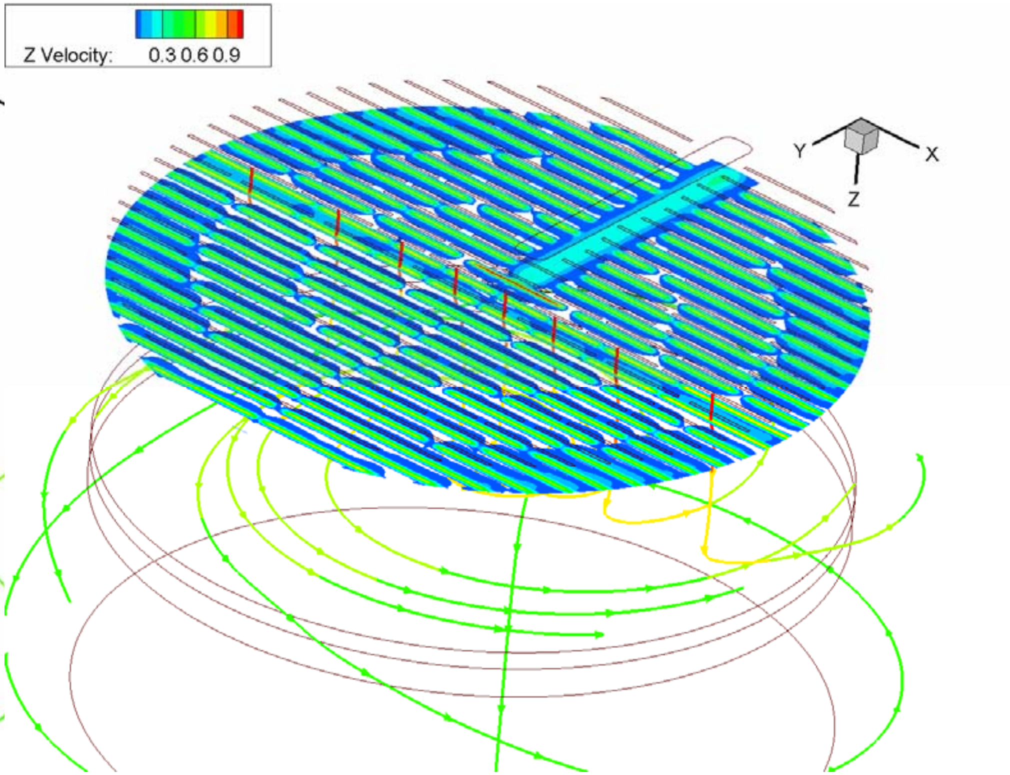
Deposition on the cold plate (black area on the photograph) corresponds to the area where model predicts the recirculation pattern (white area on the modeling figure)

Flow Flange Optimization Based on CFD Modeling

Old Flow Flange

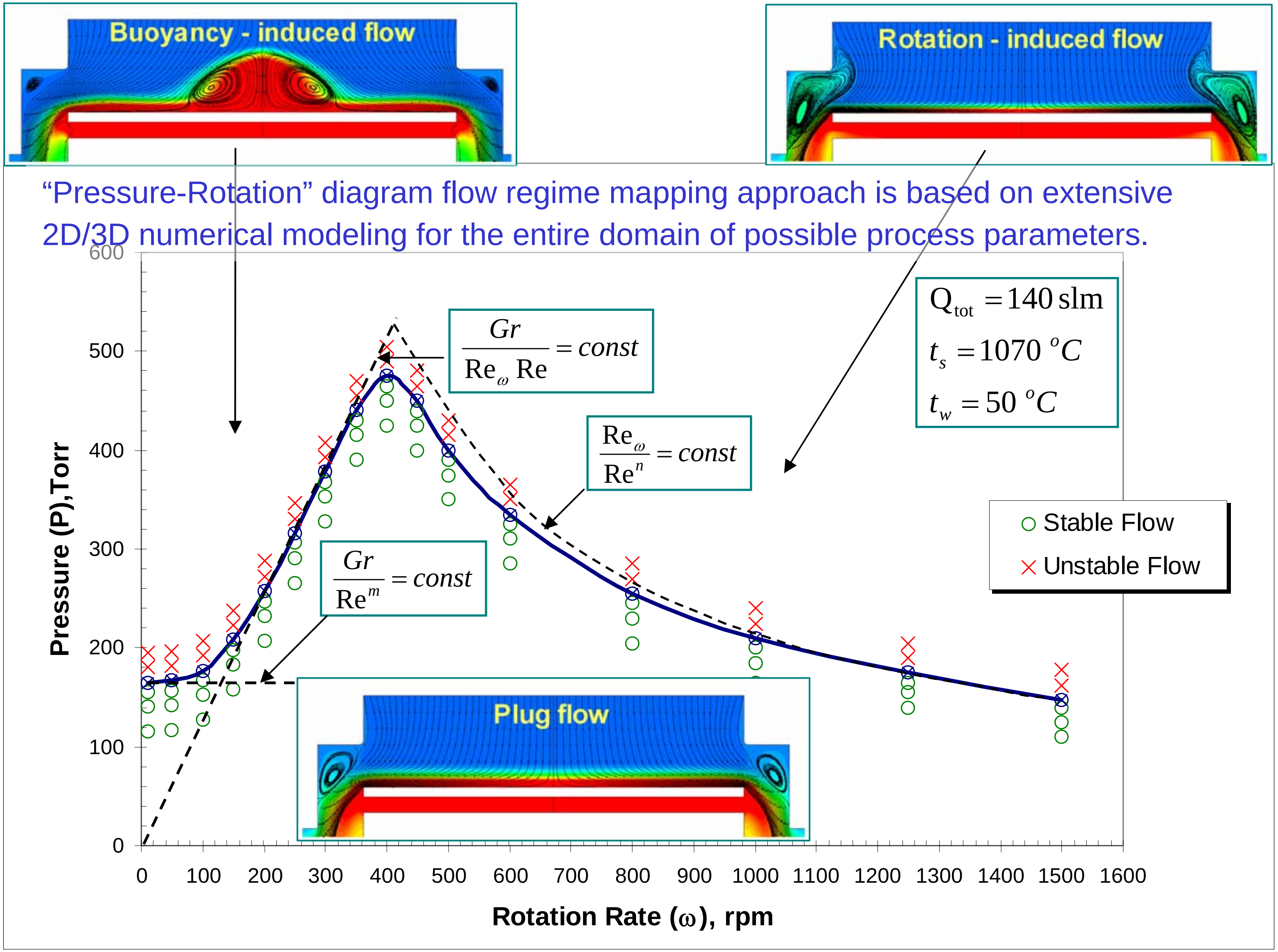


Redesigned Flow Flange



Flow Stability Mapping Approach in “$P - \omega$“ (Pressure – Rotation Rate) Diagram

“Pressure-Rotation” diagram flow regime mapping approach is based on extensive 2D/3D numerical modeling for the entire domain of possible process parameters.



$$\frac{Gr}{Re_{\omega}\,Re} = const$$

$$\frac{Re_{\omega}}{Re^{n}} = const$$

$$\frac{Gr}{Re^{m}} = const$$

$$Q_{tot} = 140\,\text{slm}$$

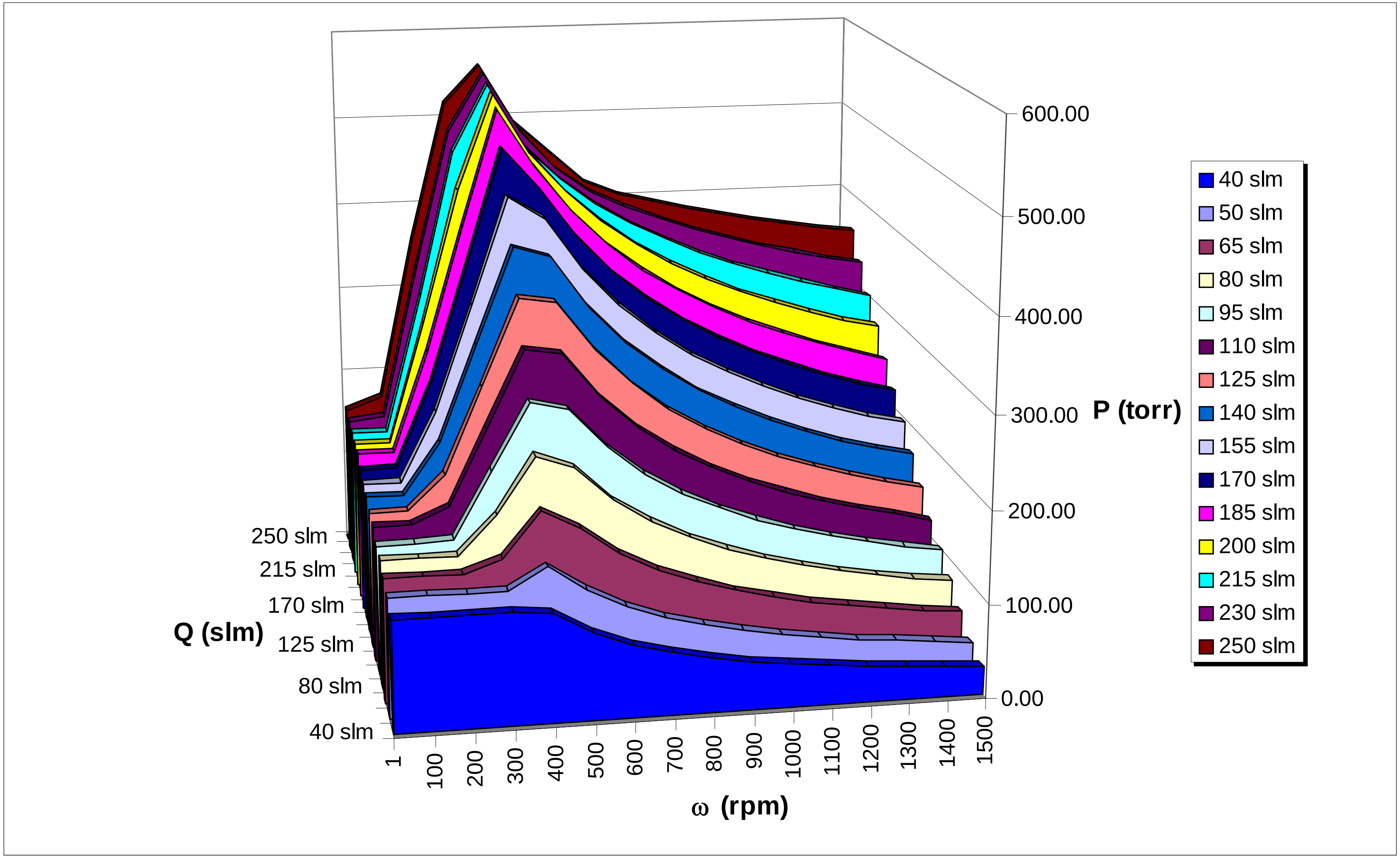
$$t_s = 1070\ ^{o}C$$

$$t_w = 50\ ^{o}C$$

"P-Q-ω" (Pressure-Flow-Rotation) Flow Stability Diagram

GaN process conditions:

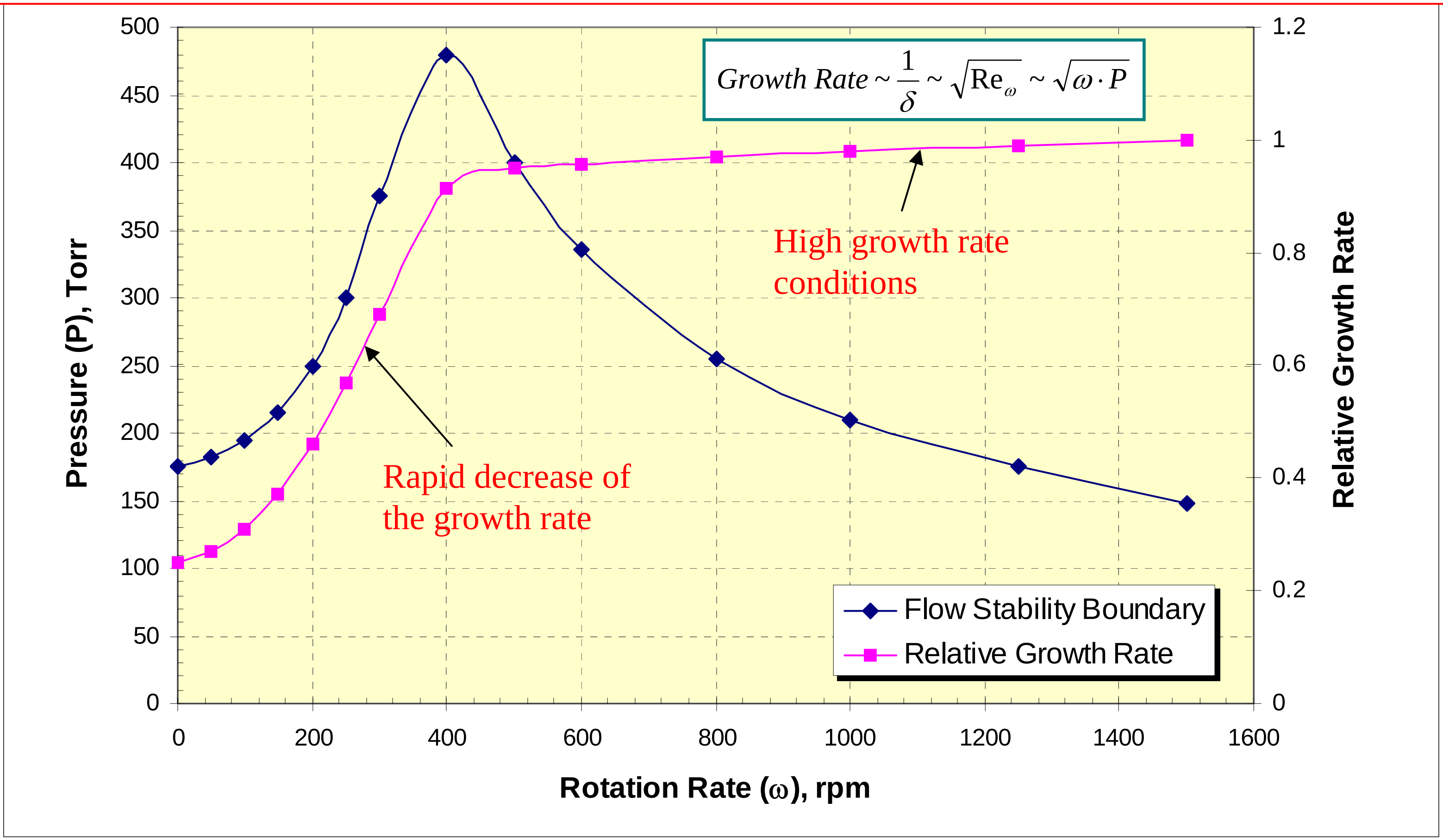
$$\frac{Q_{H_2}}{Q_{N_2}} = 4;\ \frac{Q_{H_2}}{Q_{NH_3}} = 2;\ t_s = 1070\ ^oC;\ t_w = 50\ ^oC$$



Flow Stability Map and Relative Growth Rate

GaN process conditions: $Q_{tot} = 140\ slm;\ \frac{Q_{H_2}}{Q_{N_2}} = 4;\ \frac{Q_{H_2}}{Q_{NH_3}} = 2;\ t_s = 1070\ ^oC;\ t_w = 50\ ^oC$

For the case of an infinitely large disc under mass transfer limited growth conditions the growth rate is inversely proportional to the boundary layer thickness and primarily depends on rotation rate and operating pressure.



$Growth\ Rate \sim \frac{1}{\delta} \sim \sqrt{\mathrm{Re}_{\omega}} \sim \sqrt{\omega \cdot P}$

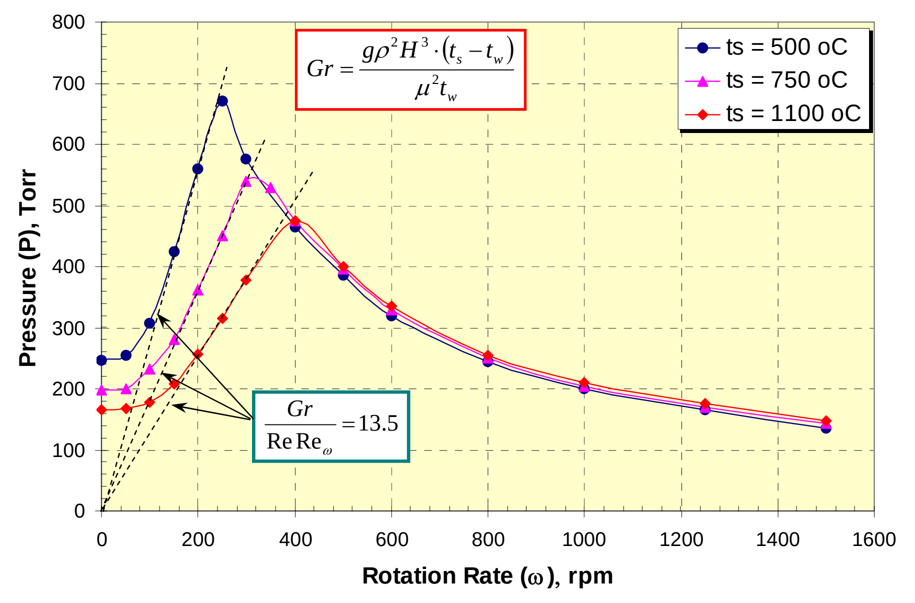
High growth rate conditions

Rapid decrease of the growth rate

Criteria for the onset of buoyancy-induced flow

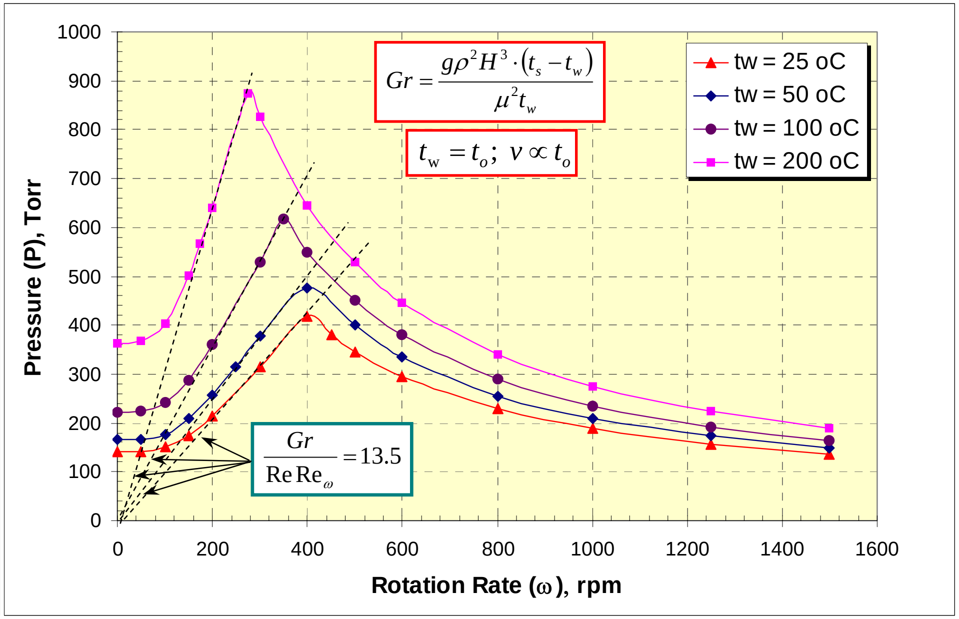
$$Q_{\text{tot}} = 140\ slm;\ \frac{Q_{H_2}}{Q_{N_2}} = 4;\ \frac{Q_{H_2}}{Q_{NH_3}} = 2;\ t_w = t_o = 50\ ^oC$$

By decreasing the temperature gradient between the wafer carrier and the inlet, we also reduce the tendency for natural convection (lower Gr), and hence, higher operating pressures can be utilized for the same rotation rate in the buoyancy induced region.



$$Q_{\text{tot}} = 140\ slm;\ \frac{Q_{H_2}}{Q_{N_2}} = 4;\ \frac{Q_{H_2}}{Q_{NH_3}} = 2;\ t_s = 1070\ ^oC$$

Higher inlet temperature has two effects on flow stability: (1) decreases the temperature gradient between the wafer carrier and the inlet which suppresses buoyancy-induced recirculation; (2) increases the through-flow velocity, which suppresses the rotation-induced recirculation.



Conclusions

- Based on modeling results and DOE optimization, an optimal geometrical position of the alkyls zones is found for different reactor sizes, which provides the best growth rate deposition uniformity on the wafer within a wide range of process conditions.
- A new modifications of TurboDisc reactors has been designed based on the optimized injector plate.
- Detailed 3D reactor modeling from direct CAD geometry import into CFD is used to find optimal process parameters for III-Nitrides materials growth.
- Excellent qualitative and solid quantitative agreement between the modeling results and experiments is observed.
- Modeling drastically reduced the process development time to a few runs and resulted in significant improvement of growth uniformity ($\delta < 1\%$) and alkyl efficiency.

Conclusions

- ✓ Quantitative flow stability maps have been developed based on extensive 2D and 3D flow modeling for the entire domain of possible process parameters.
- ✓ It has been shown that all typical flow regime regions that can be encountered in a rotating disc reactor can be presented in a single P-ω diagram, which also transparently captures the effects of all other process parameters.
- ✓ New dimensionless criteria have been proposed (based on Grashof, Reynolds and rotational Reynolds numbers) for defining a boundary between stable and unstable flow regimes.
- ✓ The obtained stability criteria have both fundamental and practical significance, and allow one to predict the process window that is free of both thermal and rotation induced recirculation, without performing additional numerical modeling or costly experiments.