# APPLICATION OF BARRACUDA® IN THE GAS PHASE POLYMERIZATION PROCESS

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CHEMISTRY THAT MATTERS™

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SECTION 1

# INTRODUCING SABIC

# SABIC IN NUMBERS

1976, our beginning
39 years of growth

3rd largest global diversified chemical company*
116th largest public company in the world*

91 B$ total assets
50 B$ annual revenue
6.2 B$ net income

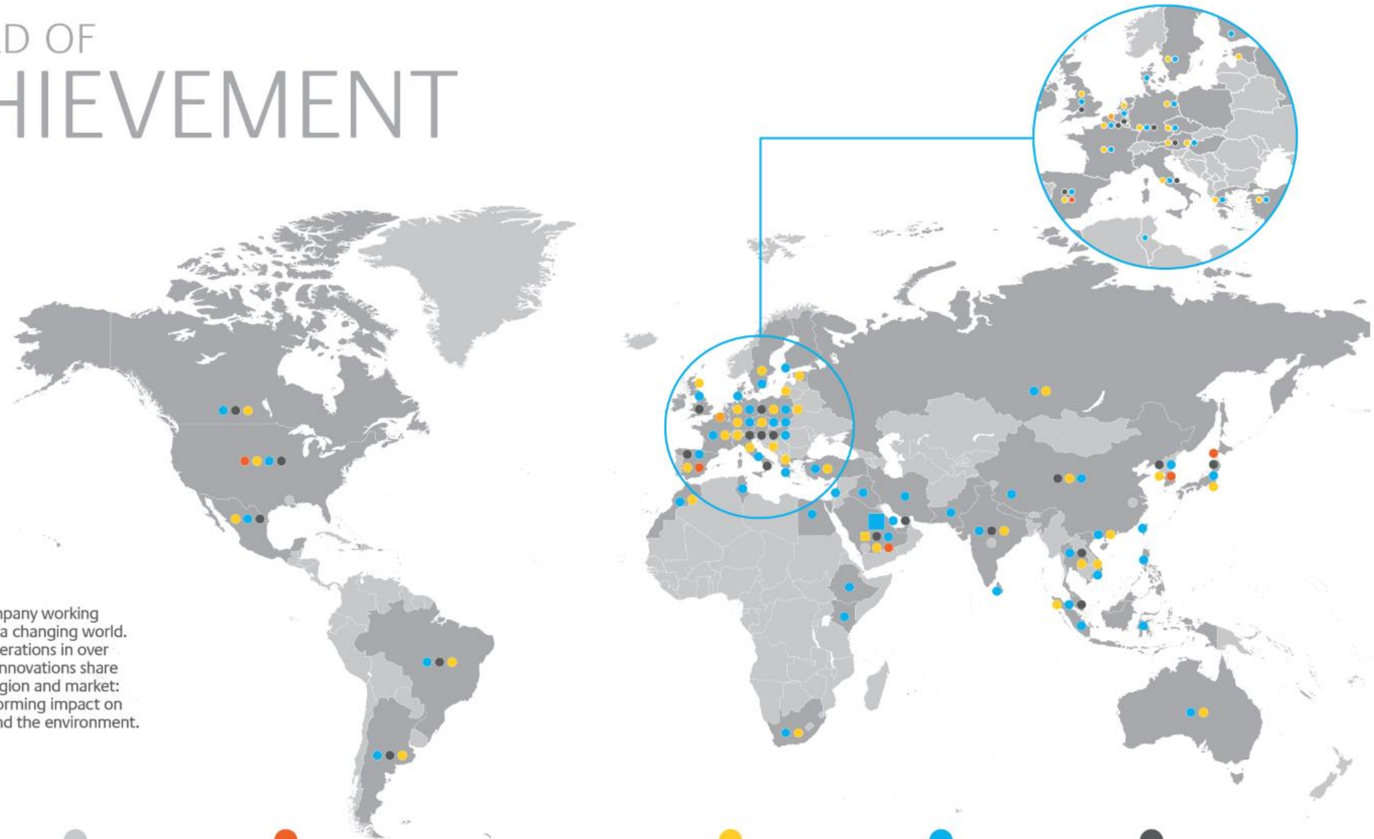
40,000 employees
50 countries
5 Strategic Business Units

64 world-class plants worldwide
5 key geographies with innovation hubs
150 new products each year
10,640 global patent filings

* Forbes 2015

# OUR GLOBAL OPERATIONS

## A WORLD OF ACHIEVEMENT



SABIC is a global company working on the challenges of a changing world. We have business operations in over 50 countries. SABIC innovations share one thing in every region and market: a positive and transforming impact on the lives of people and the environment.

**GLOBAL HEADQUARTER**
Kingdom of Saudi Arabia

**SABIC CORPORATE RESEARCH AND INNOVATION CENTERS**
Kingdom of Saudi Arabia

**TECHNOLOGY CENTERS**
China, India, Netherlands, Saudi Arabia, USA

**APPLICATION CENTERS**
Japan, Saudi Arabia, South Korea, Spain, USA

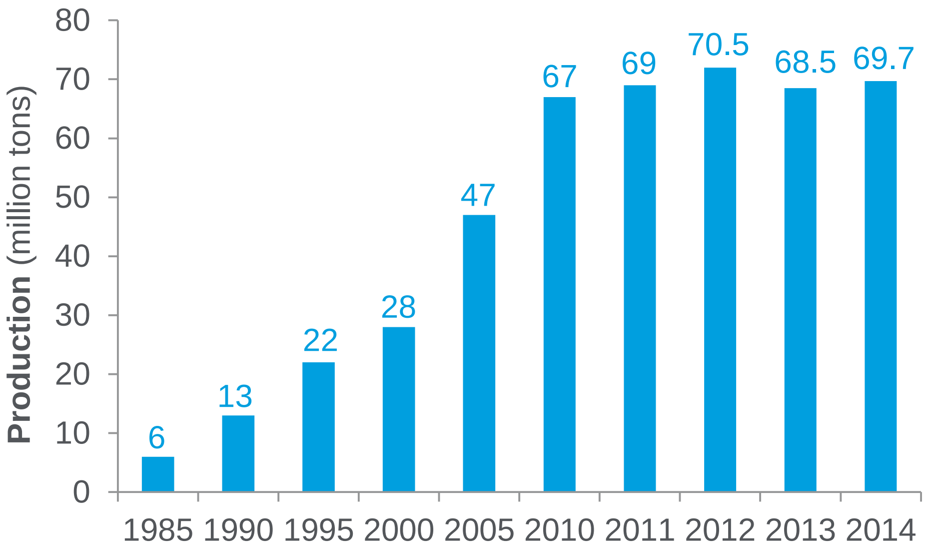
**DISTRIBUTION STORAGE FACILITIES AND LOGISTICAL HUBS**
Argentina, Australia, Austria, Belgium, Brazil, Canada, China, Czech Republic, Estonia, France, Germany, Greece, Hong Kong, Hungary, Italy, India, Japan, Malaysia, Mexico, Morocco, Netherlands, Poland, Russia, Saudi Arabia, Singapore, South Africa, South Korea, Spain, Sweden Thailand, Turkey, UK &Northern Ireland, USA, Vietnam

**INTERNATIONAL SUBSIDIARIES AND SALES OFFICE**
Argentina, Australia, Austria, Belgium, Brazil, Canada, China, Czech Republic, Denmark, Egypt, Ethopia, Finaland, France, Germany, Greece, Hungary, India, Indonesia, Iran, Iraq, Italy, Japan, Kenya, Lebanon, Malaysia, Mexico, Morocco, Nepal, Netherlands, Pakistan, Poland, Russia, Saudi Arabia, Singapore, South Africa, South Korea, Spain, Sri Lanka, Sweden, Taiwan, Thailand, Tunisia, Turkey, UK &Northern Ireland, United Arab Emirates, USA, Vietnam

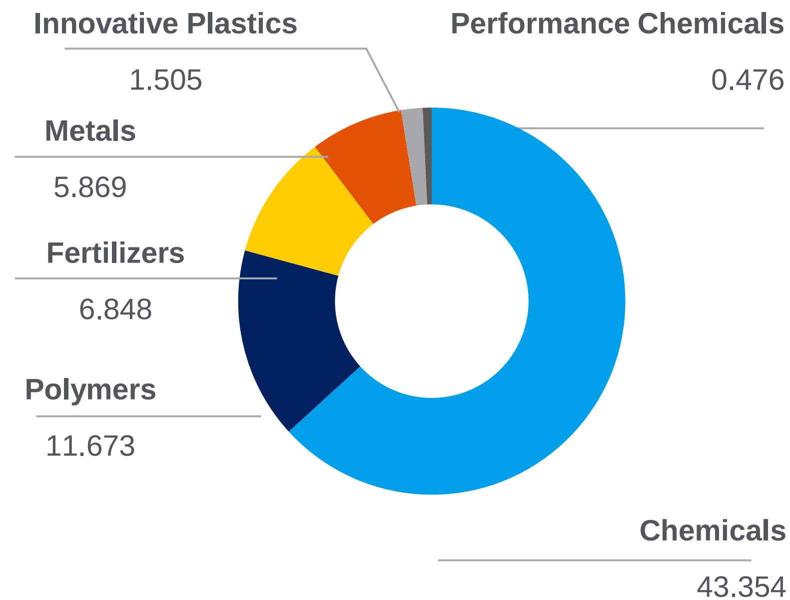
**MANUFACTURING AND COMPOUNDING COMPANIES**
Argentina, Austria, Bahrain, Belgium, Brazil, Canada, China, Germany, Italy, India, Japan, Netherlands, Malaysia, Mexico, Saudi Arabia, Singapore, South Korea, Spain, Thailand, Tunisia, Turkey, UK &Northern Ireland, USA

# RAPID GROWTH

## A high rate of growth…




## …reaching 69.7M metric tons in 2014



# WE RANK AMONG THE TOP PRODUCERS WORLDWIDE

## #1

Mono-ethylene glycol

MTBE

Polycarbonate

Polyphenylene ether

Polyether imide

## #2

Methanol

## #3

Polyethylene

Polypropylene

Polybutylene terephthalate

Engineering plastics
and its compounding

# GROUNDED IN SOCIAL RESPONSIBILITY

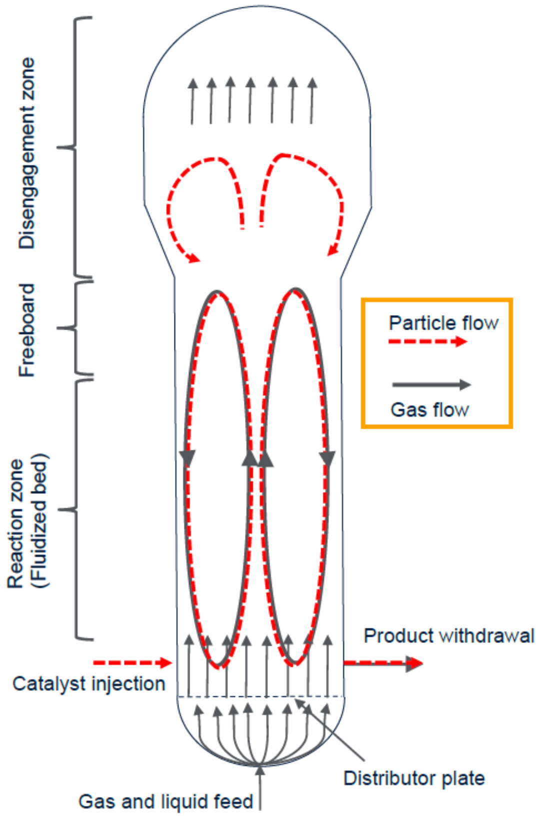
The wellbeing of our people, our stakeholders, and the communities and environments in which we operate is a business objective and a goal in its own right.

- Investing in responsible supply chain and manufacturing solutions that reduce environmental impact
- Working with customers to develop sustainable products and processes
- Supporting local and regional communities worldwide with financial assistance and employee volunteering
- Maintaining an outstanding record of health and safety in all our industrial operations

SECTION 2

# GAS-PHASE POLYMERIZATION IN FBR’S

# FLUIDIZED BED REACTOR




- PSD: 20-80µm (catalyst)
  100-5000µm (polymer)
- Operation: >60°C, > 25 bar
- Reaction zone - where fluidization occurs
  - 10-15m high
  - L/D~2.5-5
- Disengagement zone:
  - gas leaves at the top of the reactor
  - solids and gas separate
  - fluidized particles return to the dense section and are discharged from the bottom
  - $D_{DZ} > 2 \times D_{Rx.}$
- Superficial gas velocity - 0.5-1 m/s
- Pulsed catalyst feed and product withdrawal

Advantages:

- Continuous process
- Dry or condensed mode (liquid recycle)
- Extended product range

SECTION 3

# CPFD MODELLING APPROACH

# BARRACUDA VIRTUAL REACTOR® MODEL OVERVIEW

# MODEL FEATURES AND KEY ASSUMPTIONS

- Models were created to provide a fundamental understanding of the system behavior as a function of process conditions

- Models included gas, liquid and particle dynamics, non-isothermal conditions, polymerization reaction, evaporation and condensation

- Simplified reaction scheme was implemented to approximate polymerization reaction and include heat of polymerization in the heat balance

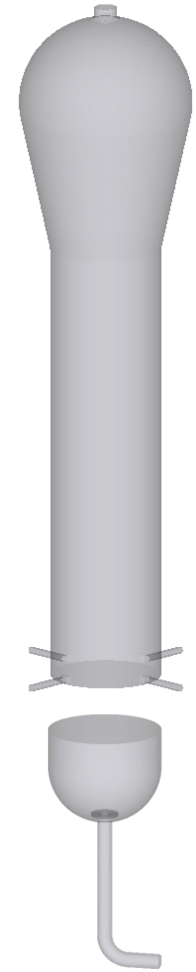
- Separate reactor and bottom head (BH) models were used
  - Radial distribution of liquid mass flux from the top of the BH model (assuming radial symmetry) used as point-source injection in the reactor

- Fresh catalyst feed was ignored

- Walls were assumed to be adiabatic with no heat losses

- Particle shape effects, and sticking effects due to particle material, static electricity or liquid films, were neglected

- Vapor-liquid equilibrium was calculated by Raoult's Law



# INITIAL AND BOUNDARY CONDITIONS- BOTTOM HEAD

**Initial Conditions**

- Bottom head space contained no condensate droplets

- Pressure, temperature, and gas composition were initialized to the inlet conditions

**Boundary Conditions (BC)**

- **Pressure BC** – Pressure BC was placed at the top of the bottom head space. The estimated pressure at the bottom of the fluidized bed and a K-factor (for $\Delta P$) based on the design of the distributor plate were used.

- **Flow BC** – Cycle gas and condensate particles entered *uniformly* through the inlet pipe

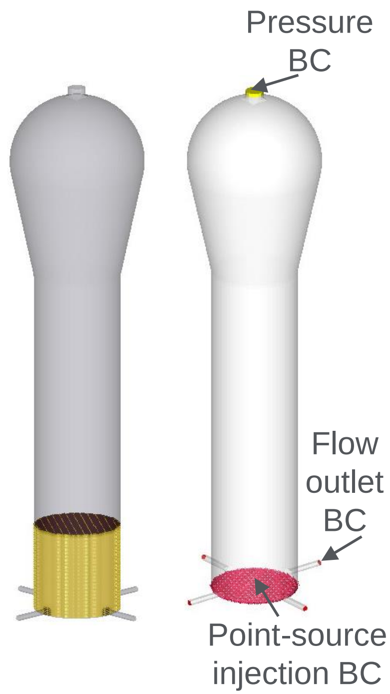
# INITIAL AND BOUNDARY CONDITIONS

**Initial Conditions**

- Fluidized bed was initially at rest with uniform pressure and temperature
- Bed of specified mass comprised polypropylene and catalyst particles

**Boundary Conditions**

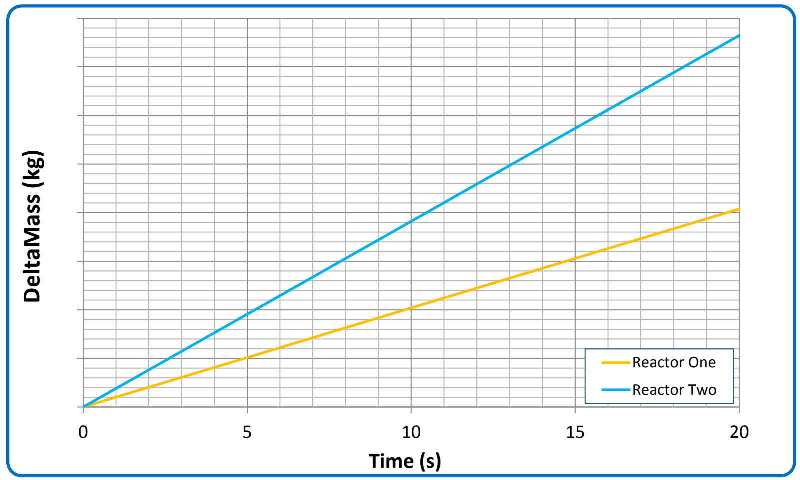
- **Pressure BC** – Outlet gas and entrained solids were allowed to leave domain through the pressure BC located at the top of the geometry. The pressure was maintained constant.
- **Injection BC** – Cycle gas was introduced *uniformly* through this flow BC located at the top of the distributor plate. Condensate particles were introduced using point-source injections and radial distribution of liquid flux computed at the top of the bottom head. Flow rates, composition, and temperatures were specified.
- **Flow BC –** "Estimated" continuous gas flow rate was specified at the product discharge boundary. Polypropylene, catalyst and condensate particles were allowed to leave domain through the boundary.



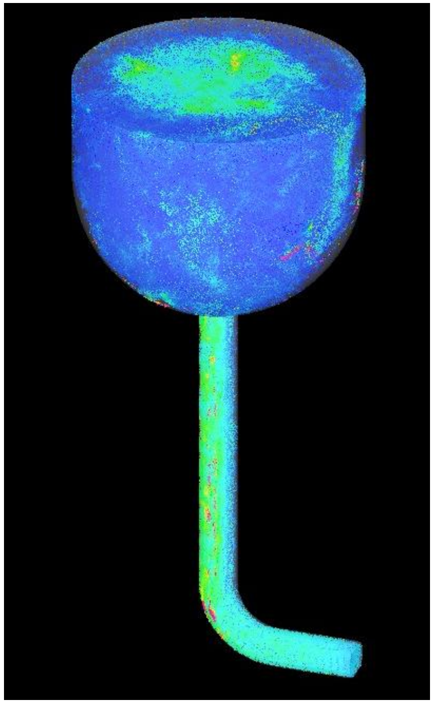
# POLYMERIZATION KINETICS VALIDATION

- The polymerization reaction was validated by simulating each reactor with the following assumptions to isolate the effect of polymerization reaction on bed mass:
  - Isothermal operation
  - Condensate flow assumed to be vaporized on entry (no condensate droplets)
  - No outflow of gas or solids allowed through the product discharge boundary
- Under these conditions, the bed mass increase was due to the production of polypropylene. The rate of increase compared well with the targeted values.

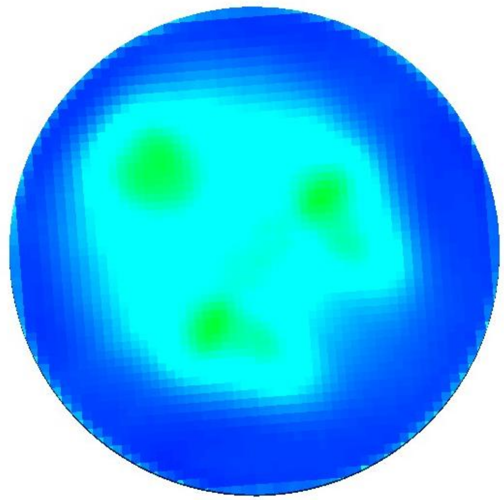
| Increase in Bed Mass | | |
|---|---|---|
| **Reactor** | **Target (MT/hr)** | **Simulated (MT/hr)** |
| One | X | X |
| Two | Y | 0.97 Y |



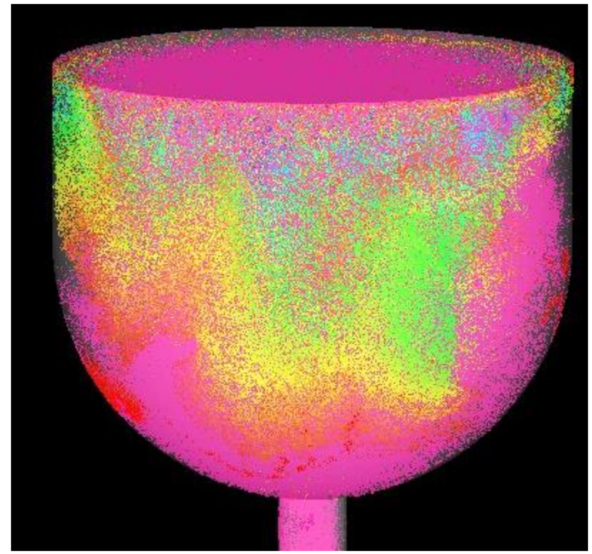
# BOTTOM HEAD RESULTS



Liquid volume fraction



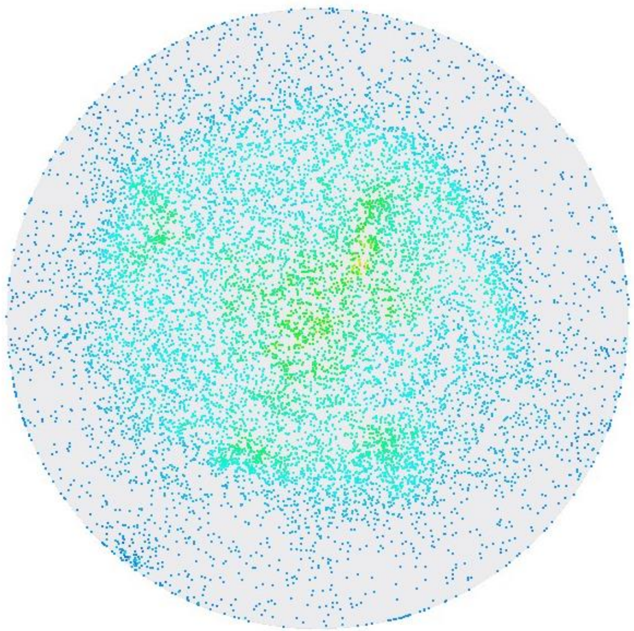
Time averaged liquid volume fraction



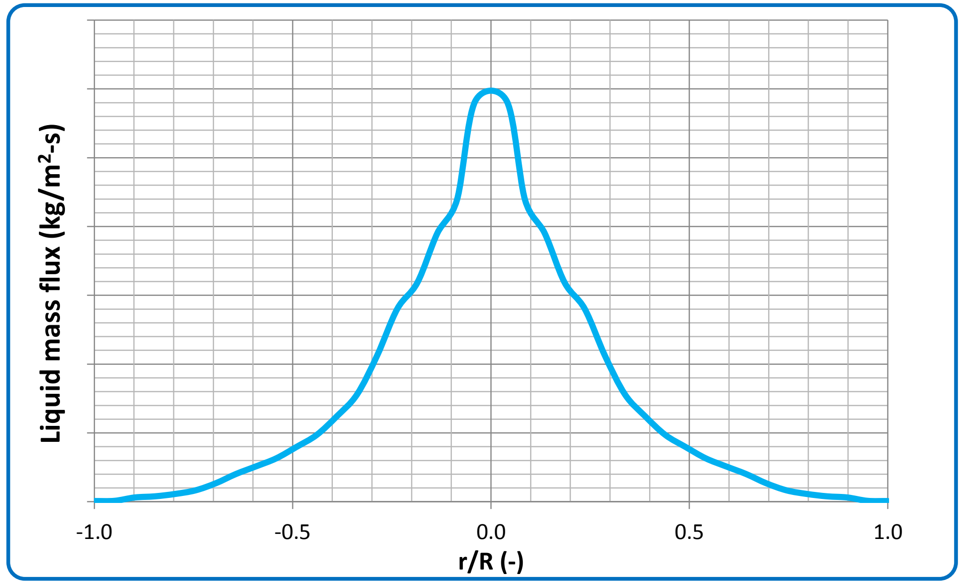
Liquid velocity (Any color other than pink shows downflow)

- **Barracuda computed liquid-rich region near the center and liquid-lean region near the walls, at the distributor plate**
- **The code also computed downflow of liquid near the walls, in the bottom head**

# BOTTOM HEAD RESULTS

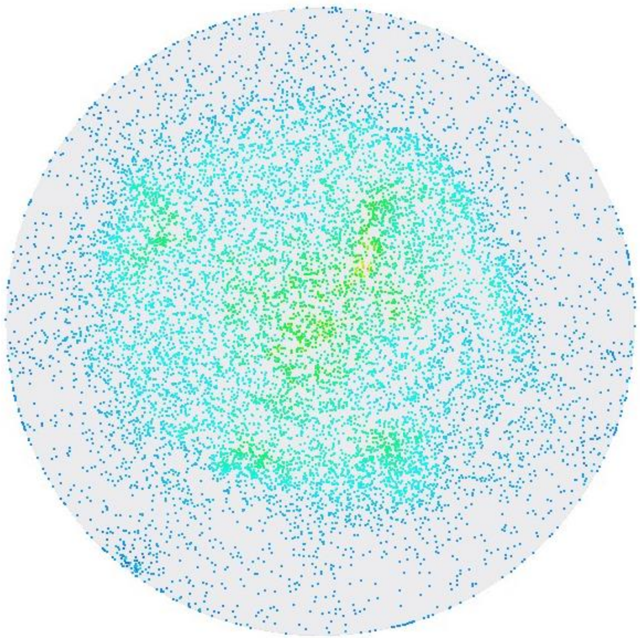


Liquid flux at the distributor



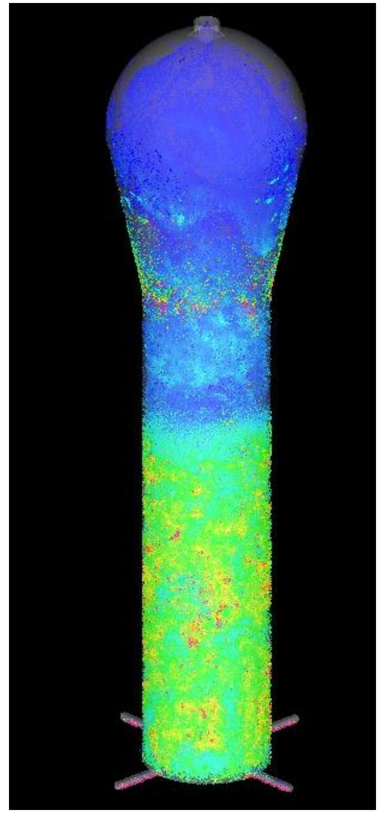

- **Histogram was used to determine radial distribution of liquid flux at the distributor plate**

# REACTOR HYDRODYNAMICS & PRODUCT DISCHARGE



Liquid flux at the distributor

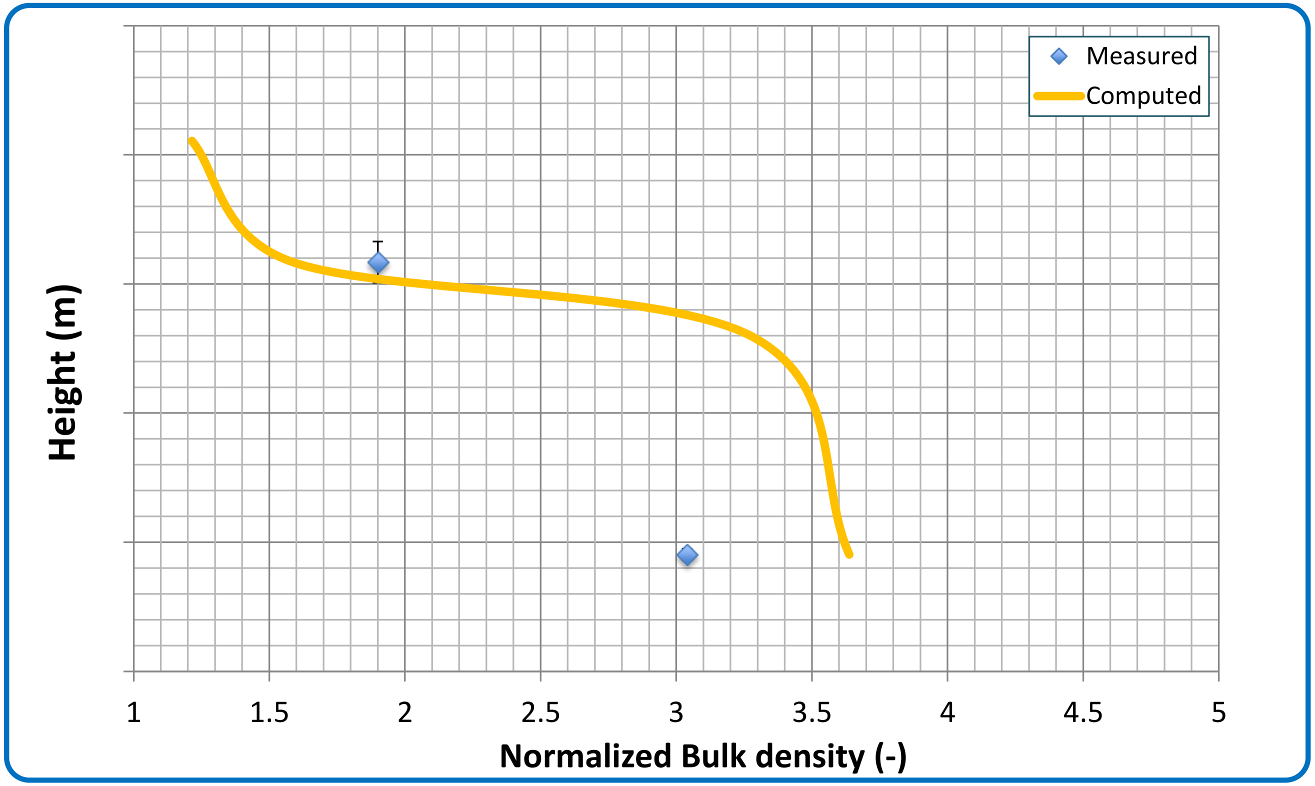
Input for feed to the reactor



Product discharge composition

- **Reactor model was utilized to simulate hydrodynamics, reaction kinetics and product discharge**
- **The current method for the analysis of product discharge, including outlet composition and hydrodynamics at the bottom of the reactor, needs improvement, as it does not represent a real system**

# BULK DENSITY VERIFICATION




- Barracuda predicted the freeboard bulk density reasonably well, but under-predicted it in the dense bed

SECTION 4

# PROS & CONS AND CHALLENGES

# PROS & CONS AND CHALLENGES

**Pros:**

- Fundamental insight on FBR’s – Ex.: Acrylonitrile, Gas-phase polymerization
- Hydrodynamics and reaction kinetics – Ex: Ammoxidation, Polymerization, Evaporation
- Particle size distribution
- Large number of particles using E-L approach – *Computational particles*
- Point source injection
- Erosion model
- Fast GPU version
- Good support from Engineering team

**Cons:**

- Does not match bed densities well
- Flow and pressure outlet BC challenging for continuous or periodic discharge of *known flow rate of solids,* at the bottom of the reactor
- Particle collisions are modelled
- No manual
- Insufficient customization options
- Separate CAD Software required
- No User Defined Function (UDF)
- Limited post-processing capabilities within GMV – *EnSight or Python*

SECTION 5

# CONCLUSIONS AND OUTLOOK

# CONCLUSIONS AND OUTLOOK

- Barracuda® provided fundamental insight into the behavior of bottom head and reactor
  - Liquid distribution and flow behavior in the bottom head
  - Hydrodynamics and product discharge composition in the reactor
- Improved method for simulating product discharge from the reactor will be evaluated
- Reaction kinetics model will be improved by incorporating activation energy in the form of Arrhenius equation
- 2D histogram for radial distribution of liquid flux to capture asymmetry could be considered
- Catalyst injection will be considered
- Barracuda is an effective tool when used as a means to providing engineering solutions
  - Still more work needs to be done to improve the software

SECTION 6

# ACKNOWLEDGMENTS

# ACKNOWLEDGMENTS

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Josh Taylor - SABIC

# THANK YOU - QUESTIONS

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