Polyester Digestion: VOLCAT

Summit on Realizing the
Circular Carbon Economy

IBM Almaden; San Jose, CA

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IBM Almaden Research Center

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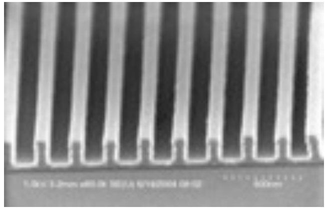
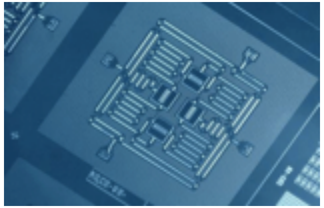
IBM

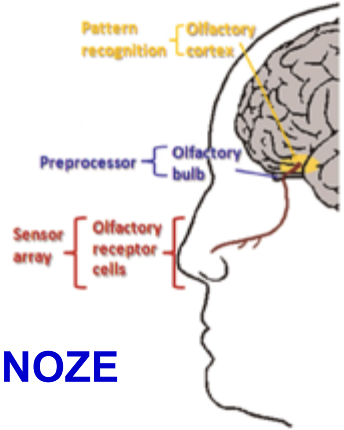
IBM Materials Innovation: Polymer Materials



Lithography/Albany



QBIT Fabrication



COGNOZE

IBM Technology

Experiment

Materials Innovation AMD

Computation/Machine Learning

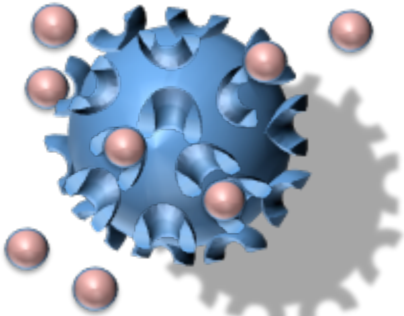
Grand Challenges

Purification Materials

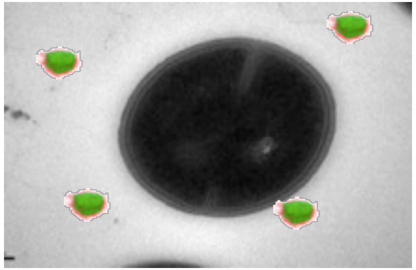
Cognitive Therapeutics

Catalysis/Green

Energy

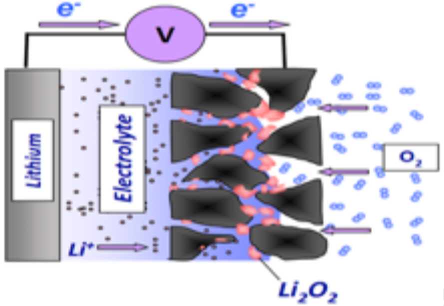


Complex Separations



Antimicrobial Polymers

PET recycling



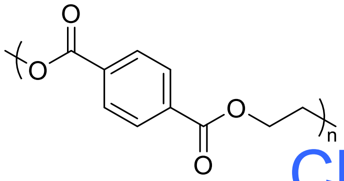
Next Gen Battery

Catalytic Polymer Recycling @ IBM

- IBM invests in polymer science research to help enable next generation computing
- Computational chemistry, materials simulation and accelerating materials discovery through AI/ Machine Learning augment our experimental work
- Catalysts have been developed for the creation and breakdown of polymers
- We've developed a molecular sorter technology for r-PET (VOLCAT)
- We are interested in demanding applications moving these technologies to the next level through partnership

Jim Hedrick

Recycling of PET (r-PET): Challenges



Mechanical Recycling

- Sorting, washing (zero contamination tolerance)
- Only “non-colored” bottles
- High Temp Processing (T > 250^{o}C)

COLOR/Low Quality

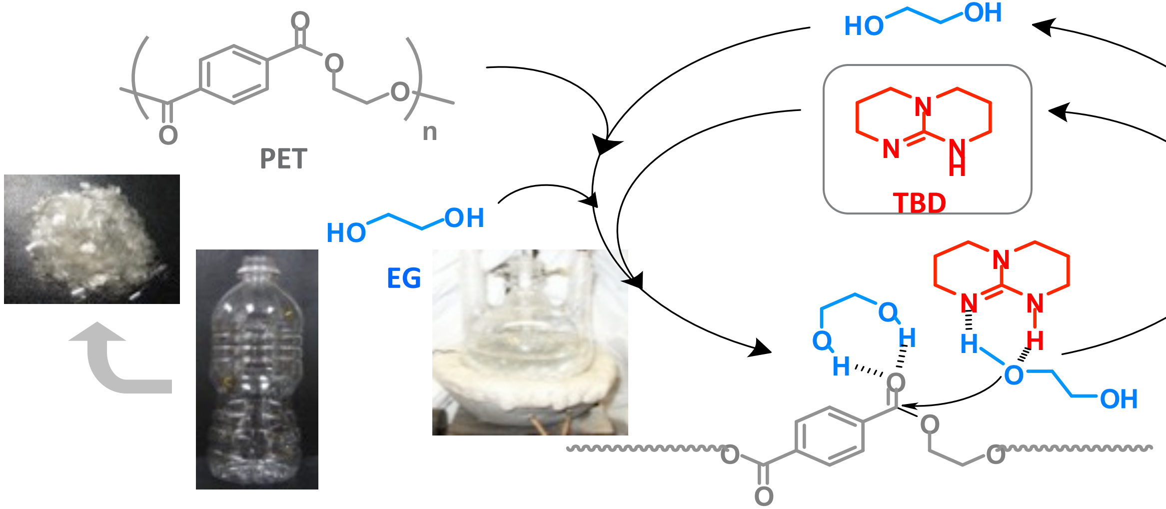
Chemical Recycling

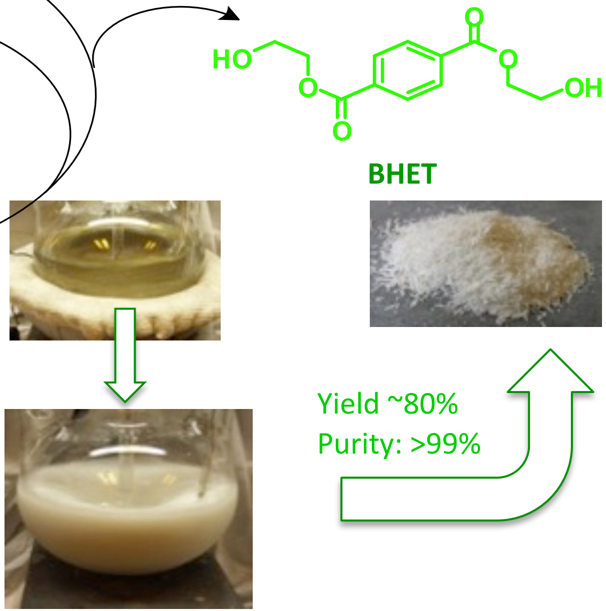
- Chemical Depolymerization
- Reaction Product (Monomer) Requires Purification for Polymerization
- Incorporated into Virgin PET Polymerization

COST

IBM’s Organocatalytic depolymerization of PET

Jim Hedrick



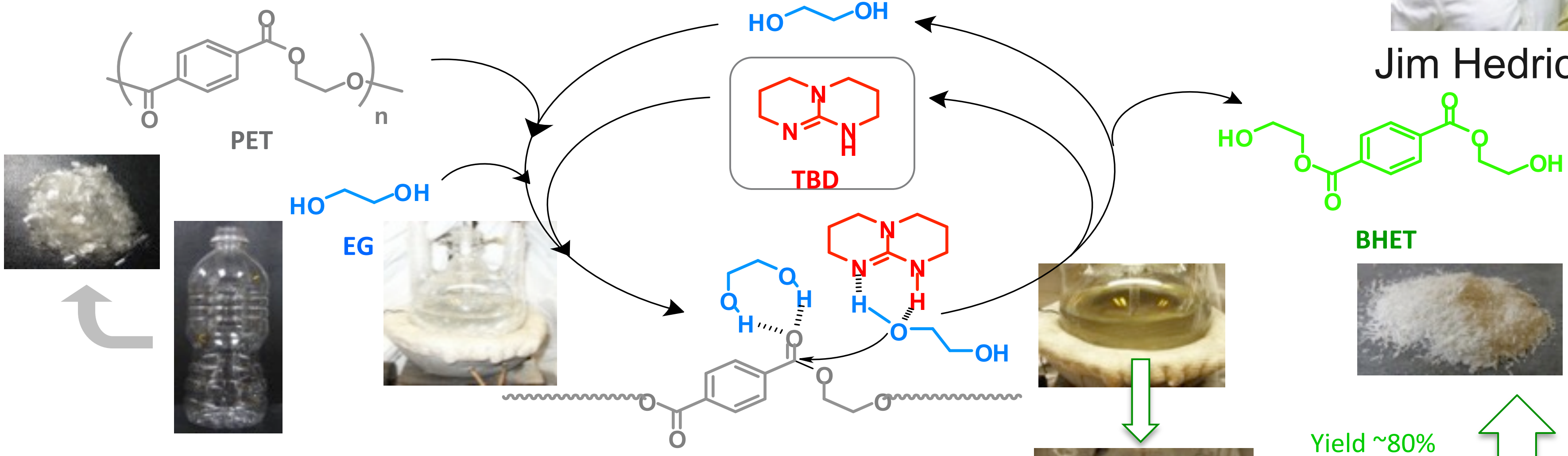


Fukushima, K; Coulembier, O.; Lecuyer, J. M.; Almegren, H. A.; Alabdulrahman, A. M.; Alsewailem, F. D.; McNeil, M. A.; Dubois, P.; Waymouth, R. M.; Horn, H. W.; Rice, J. E.; Hedrick, J.L. “Organocatalytic depolymerization of poly(ethylene terephthalate)” *J. Polym. Sci. Part A: Polymer Chem.* 2011, DOI: 10.1002/pola.24551.

IBM’s Organocatalytic depolymerization of PET

Gen 1 Catalyst: High Activity, Difficult Recovery, $$

Jim Hedrick



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IBM's PET catalytic depolymerization process (Gen 2 using DBU)

IBM's PET catalytic depolymerization process (Gen 2 using DBU)

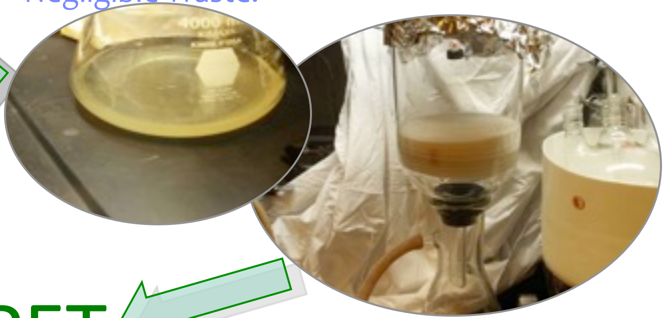
Heat to 190C, add catalyst

Cool to
Below 100C
Filter

DBU Contamination/Loss!!

Isolate BHET
(yield approx 75%)

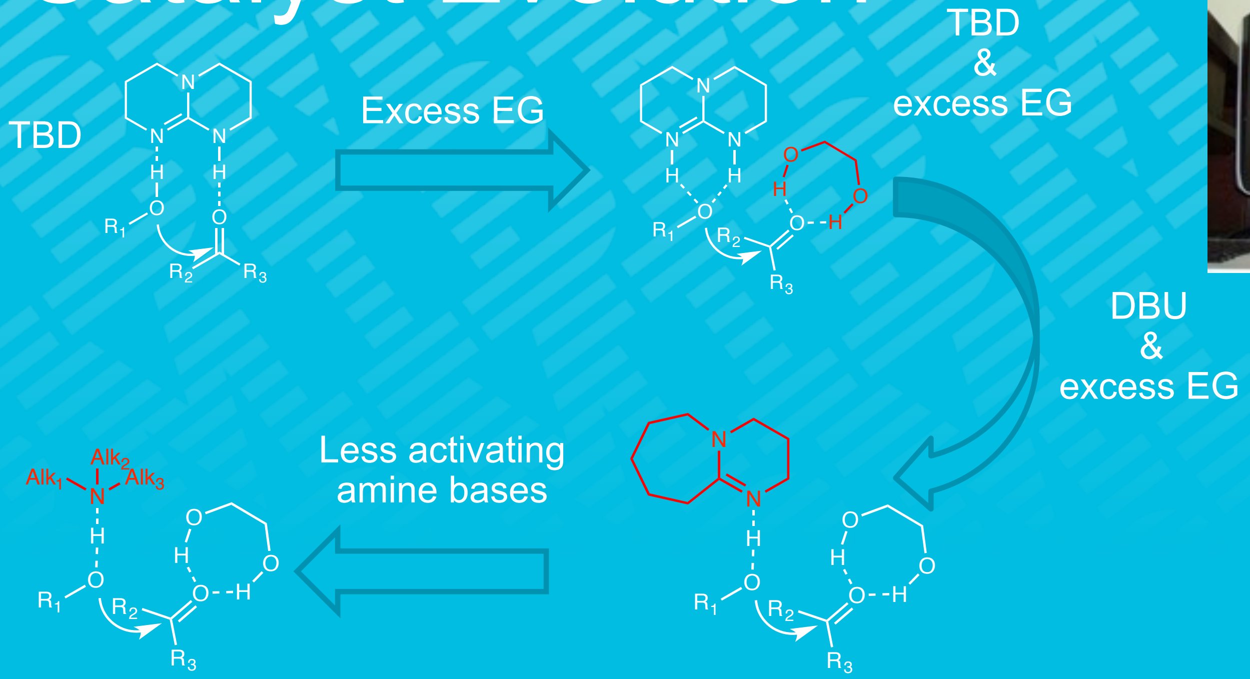
clean



Solute, to be Recycled.
Negligible Waste.

New PET

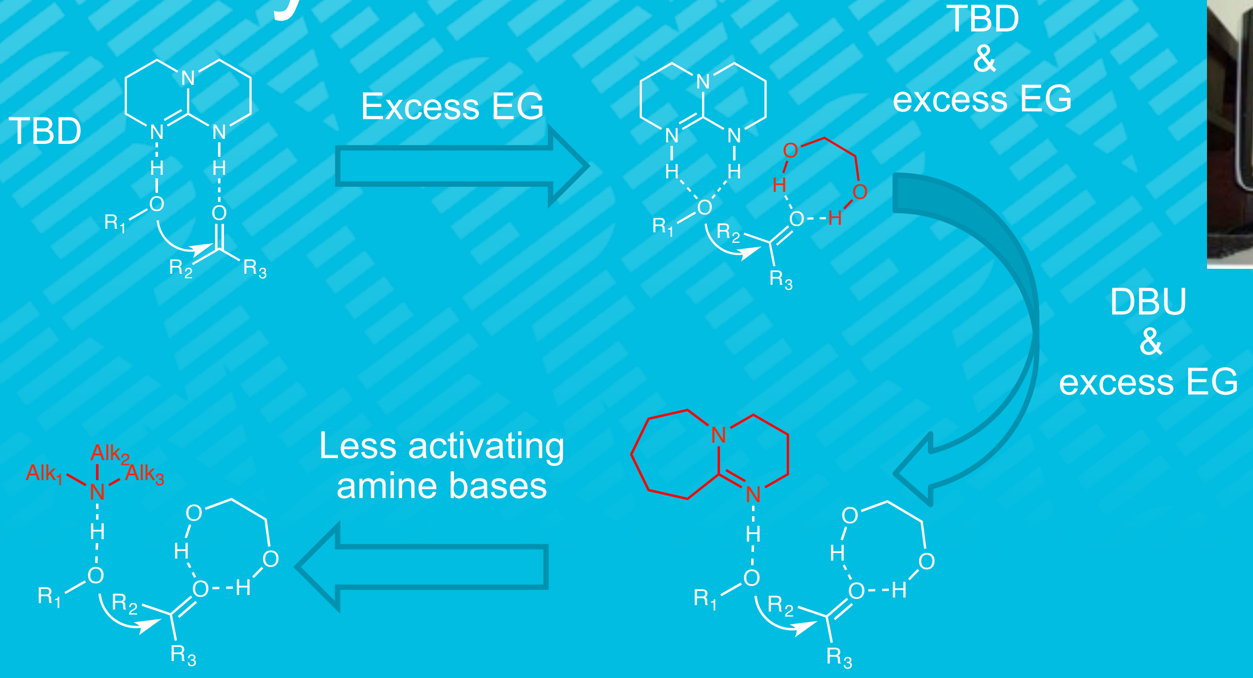
Catalyst Evolution



Gavin Jones

Computational prediction that the use of excess EG leads to a change in the mechanism allows for other types of amines to be used to catalyze PET depolymerization.

Catalyst Evolution



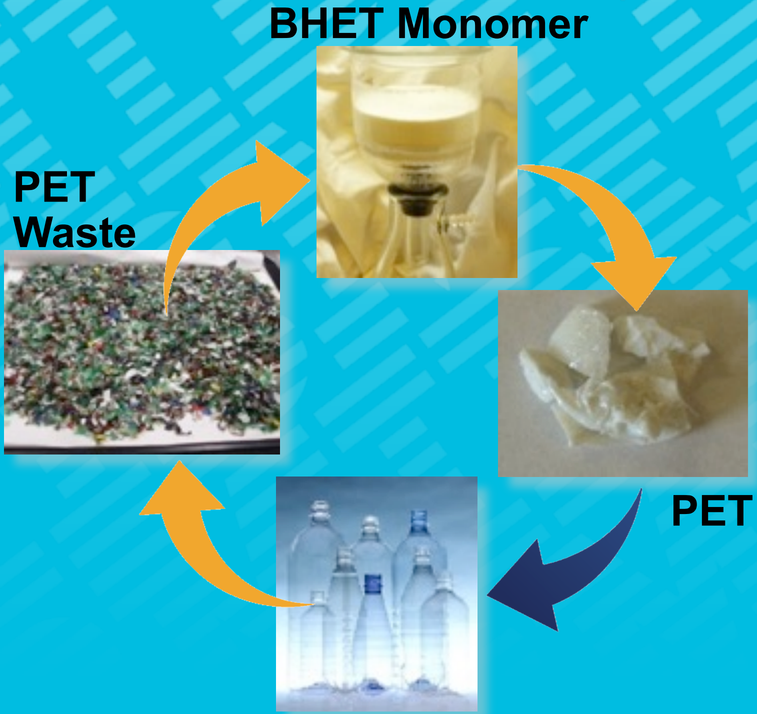
Volatile Amines?

Gavin Jones

Greg Breyta

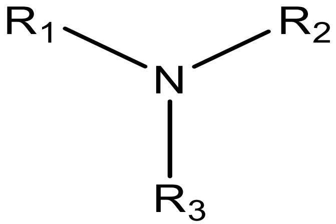
Computational prediction that the use of excess EG leads to a change in the mechanism allows for other types of amines to be used to catalyze PET depolymerization.

Volcat Technology



- Fast/Selective Catalytic Process, low temperature, easy catalyst removal/recovery
- Key Attribute– **VOLCAT is a “*Molecular Sorter*”**
    - Minimize sorting, washing and rinsing of flakes
    - Reduce/eliminate color sorting
- Outstanding results with dirty clear and mixed/colored flake inputs

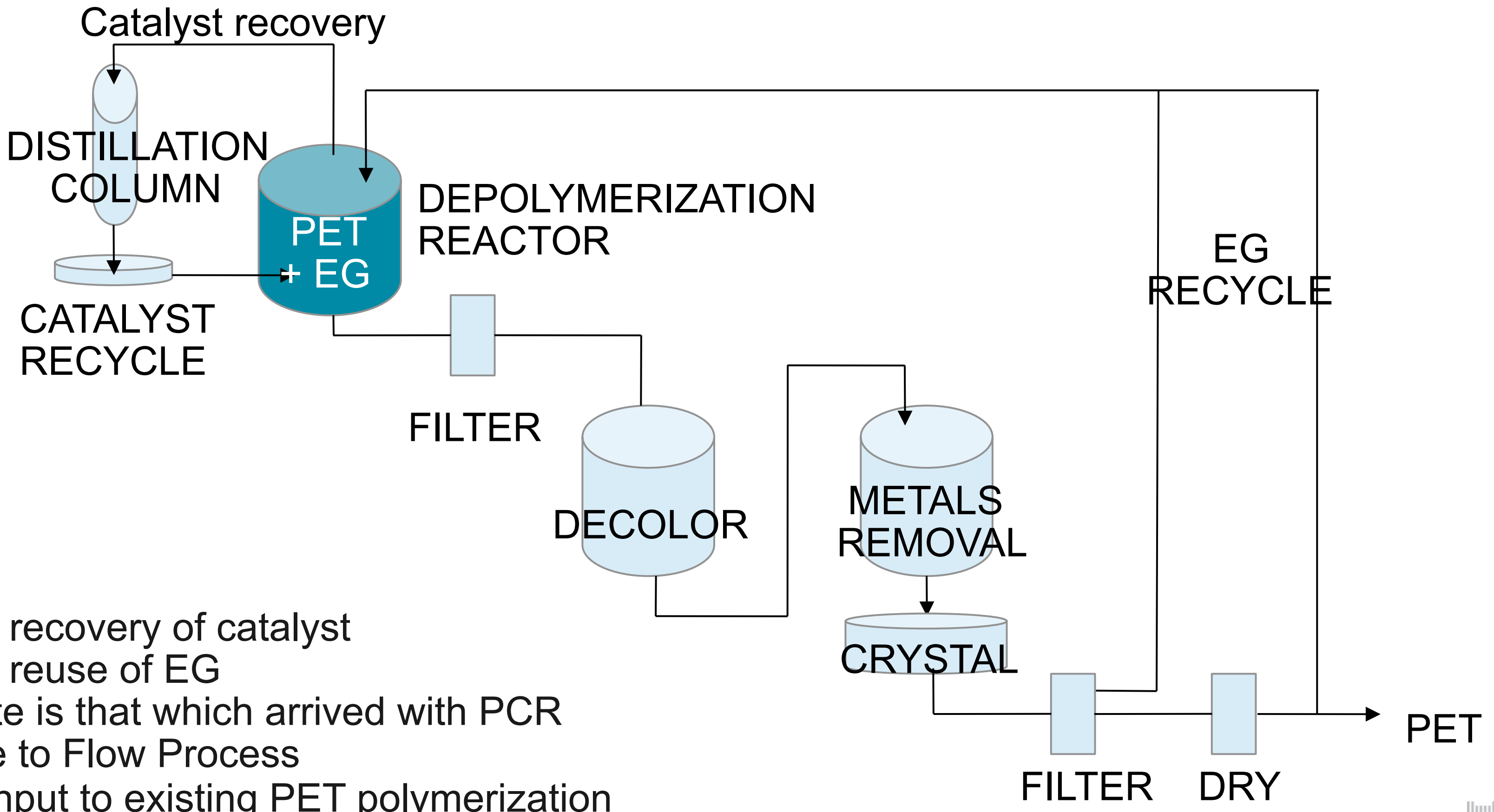
VOLCAT approach to recycled PET



- **Distinguishing Features**:
  - Volatile Catalyst is active and easily recovered;
  - Low Grade Mixed PCR PET input can produce high grade r-PET
  - Sorted Colored Flake can produce high grade r-PET

- **Economic Outlook**:
  - Lowest Cost Feedstocks and inexpensive catalyst
  - All chemicals used/recovered (no waste);
  - Low temperature/fast process
- **Other Advantages**:
  - Potential to reduce / eliminate sorting
  - Potential to reduce / eliminate washing and rinsing

VOLCAT Process Flow Today – a closed loop (as batch) process



- Complete recovery of catalyst
- Complete reuse of EG
- Only waste is that which arrived with PCR
- Adaptable to Flow Process
- Modular input to existing PET polymerization

Robust process tolerant of high degrees of contamination

Dirty Mixed Flake

Unsorted, uncleaned flake; cheap input
-A considerable amount of dirt is present (~4%)

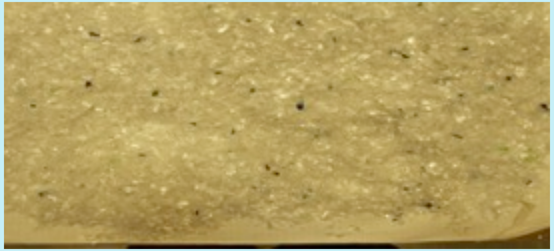
Clean Mixed Flake

All colored Flake from post-sorting/cleaning
Cheapest input – little commercial use

Dirty Mixed Flake

Worst of the worst. “Curbside pickup”
- Large amount (~8%) of “dirt” is present; cheapest input

PET/Nylon & PET/PVC flake sample

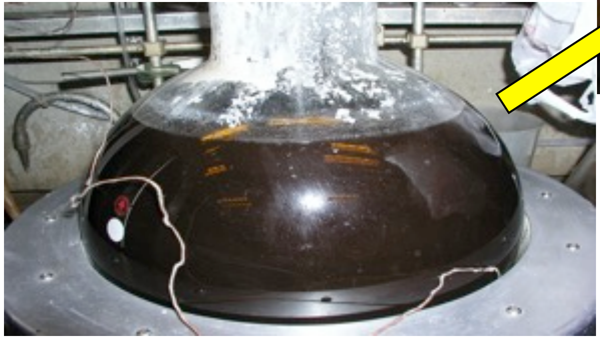


- PET flake with 3 wt% Nylon
- PET flake with 3 & 0.1 wt% PVC (NURRC + Aldrich)

VolCat Process with Clean Color Flake

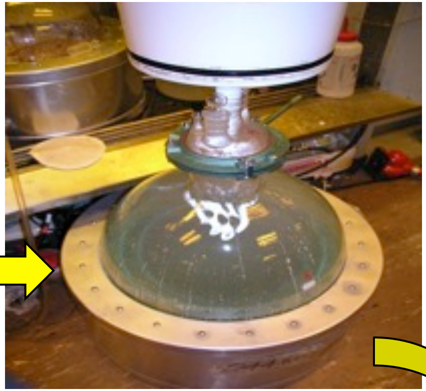
From reactor

The VOLCAT product filtered to remove this small amount of “blue stuff” (&some flake)



To give this turbid solution TO WHICH carbon was added

Filtration of carbon (left) to IX Treatment flask



Solution after post-IX filtration. Faintly blue, left to crystallize

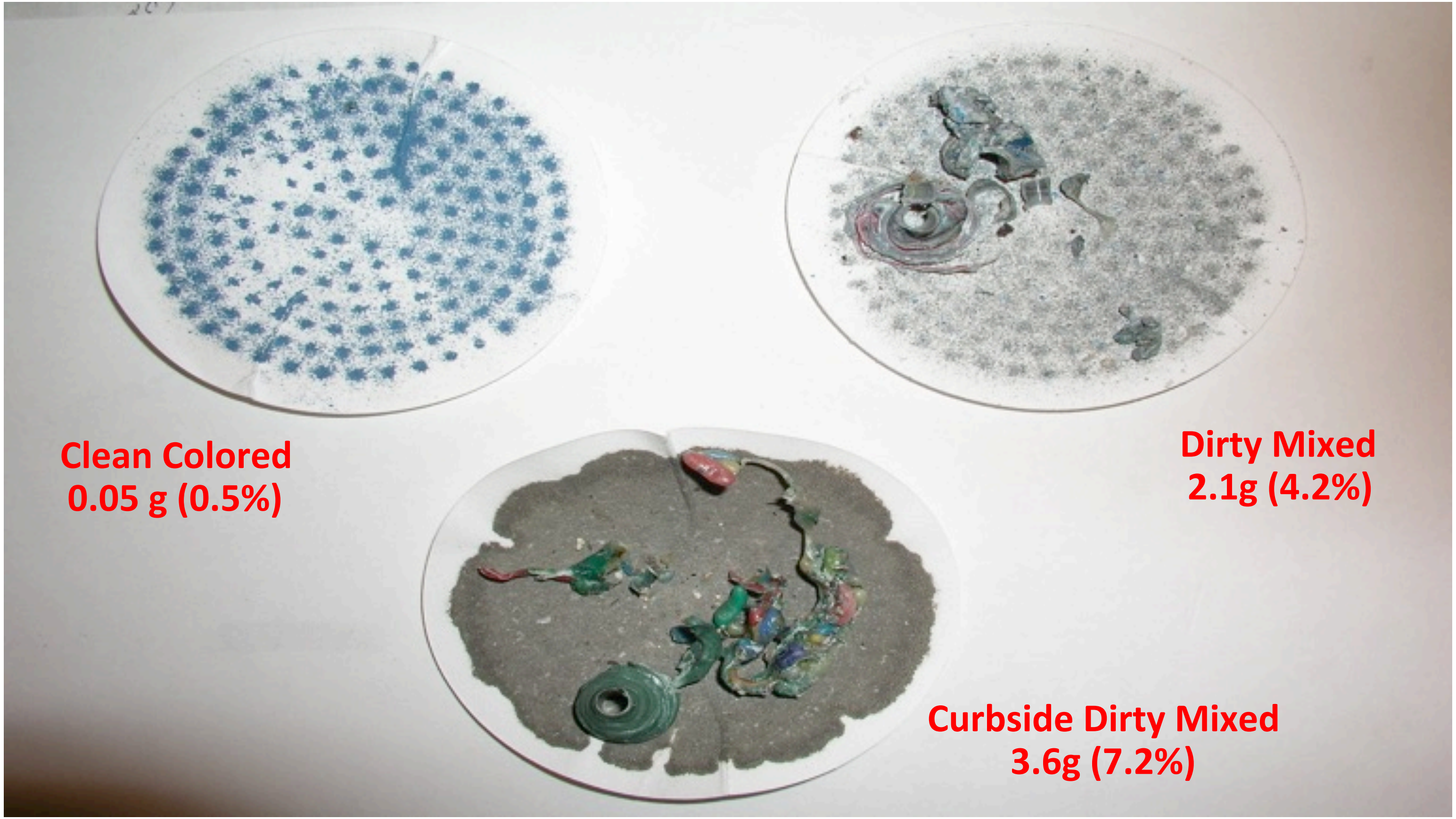
To produce this!! – Filtration next.

VolCat Processed Colored Flake (5 kg)

BHET Product
(polymerization grade)

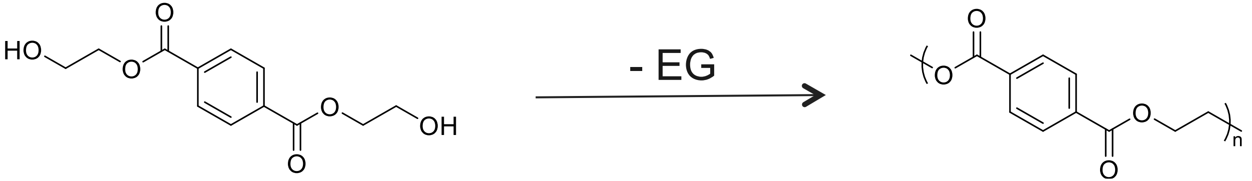
All inputs provide similar results

Filtration Step Comparison



BHET polymerization to PET*: Polymer Characterization

Any/all feeds can be "VOLCAT-ed" to produce bottle grade BHET (50%)



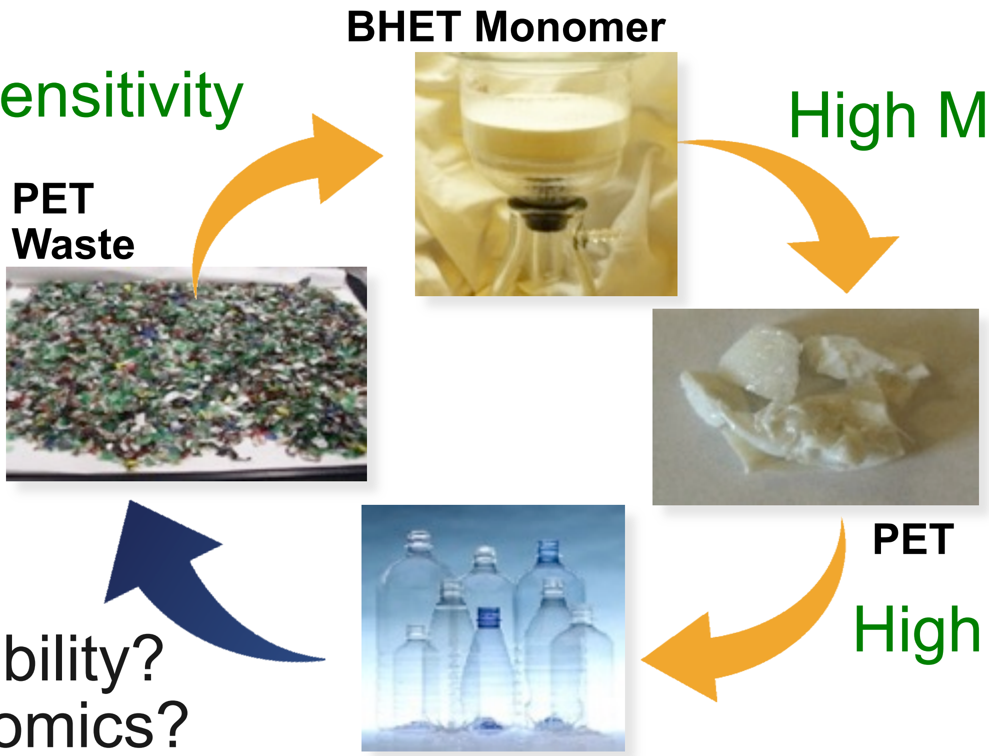
BHET Monomer Source	Transparency (L*)	Color (b*)
Virgin PET (from TPA/EG)	93	2.3
Virgin PET; Glycolysis (re-polymerized)	87	8.0
VOLCAT BHET (clean, clear flake)	93	2.1
VOLCAT BHET (dirty clear)	92	5.9
VOLCAT BHET (colored flake)	92	5.6
VOLCAT BHET (curbside, dirty)	92	4.5

* Performed by DAK Americas, an Alpek Polyester Business

PET Chemical Recycling via VOLCAT

Feedstock Insensitivity

High Monomer Purity



High Polymer Purity

Process Scalability?
Process Economics?
New Materials?

PET Chemical Upcycling via VOLCAT

Feedstock Insensitivity

PET Waste

BHET Monomer

High Monomer Purity

PET

High Polymer Purity

PET-derived AMIDE Monomers

Process Scalability?
Process Economics?
New Materials?

Catalytic Polymer Recycling @ IBM: Other Processes

- PHT Thermosets: Depolymerization at low pH
- Conversion of Poly(carbonate) to Poly(ether sulfone)

Jeannette Garcia