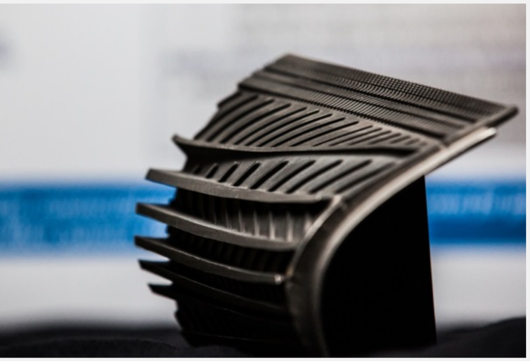
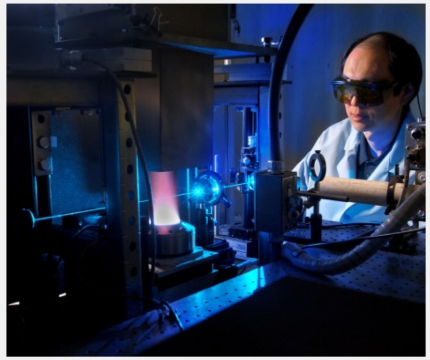
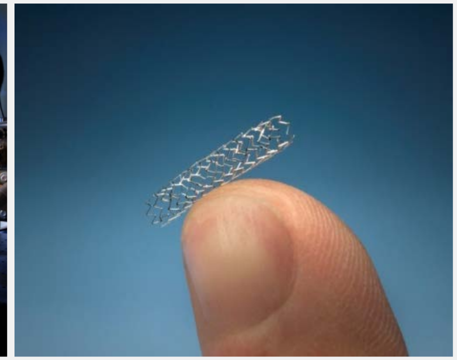
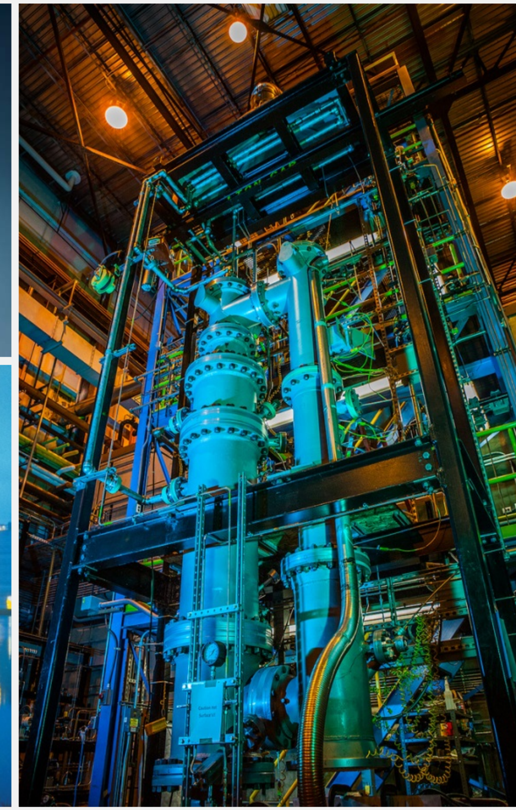
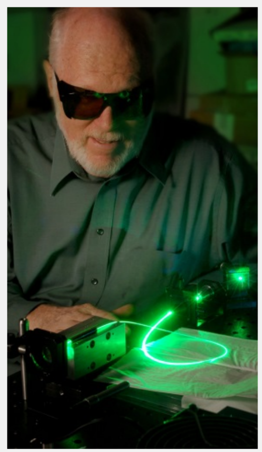
Driving Innovation ♦ Delivering Results

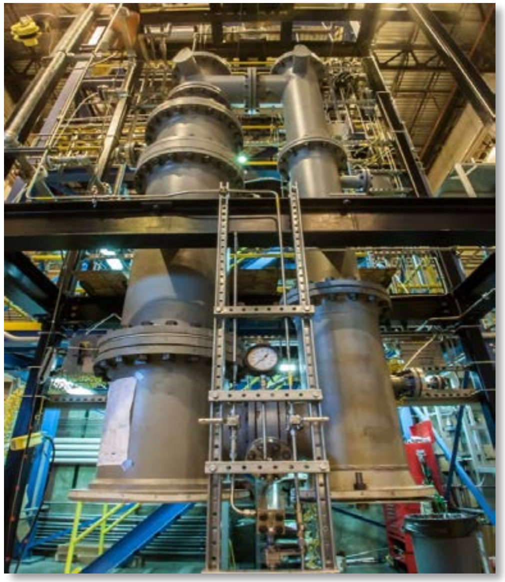

CFD modeling of the fuel reactor in NETL's 50 kw chemical looping facility

Ronald W. Breault, Justin Weber, Doug Straub and Sam Bayham.

The 41st International Technical Conference on Clean Coal & Fuel Systems

June 5-10, 2016

Chemical Looping Reactor (CLR)

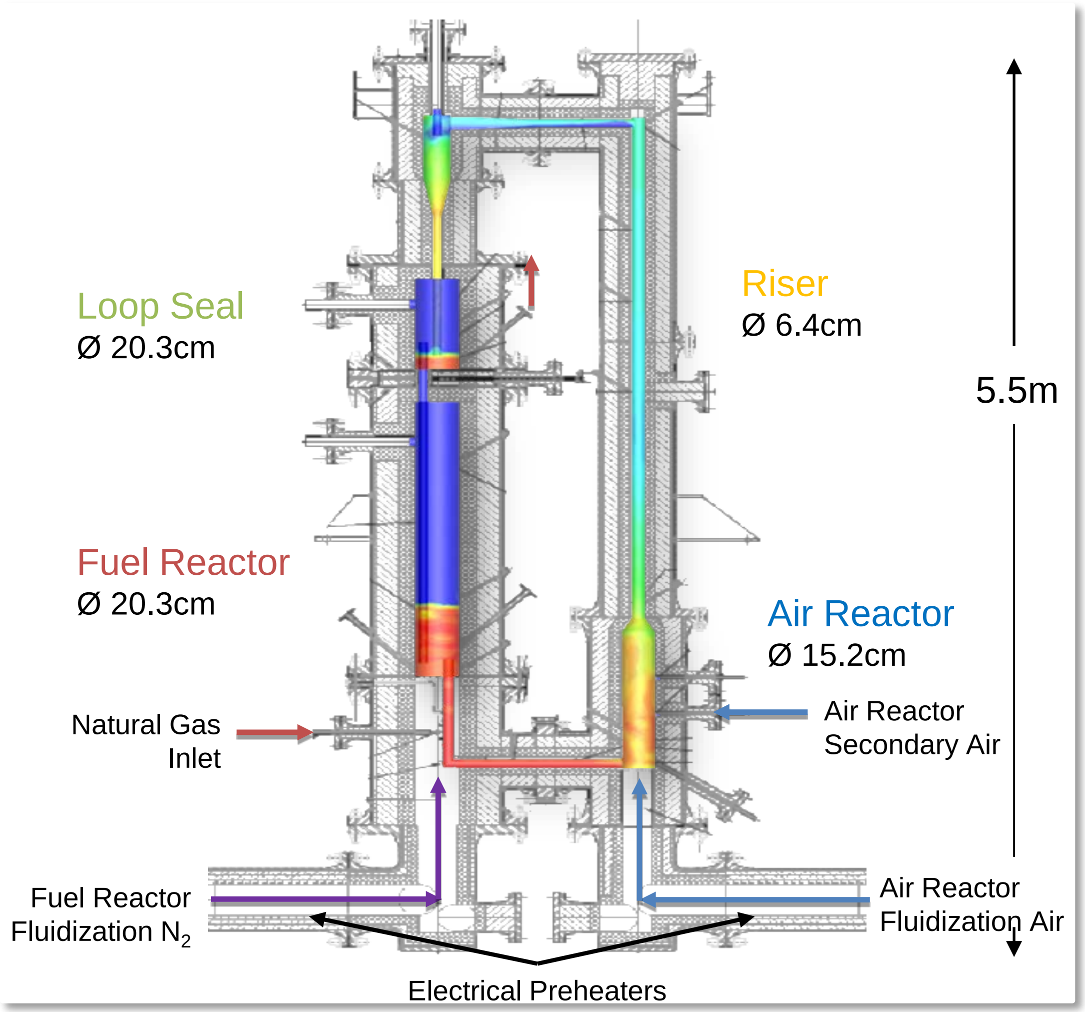


Capacity: 20-50kW$_{thermal}$

Fuel: Natural gas (CH_4)

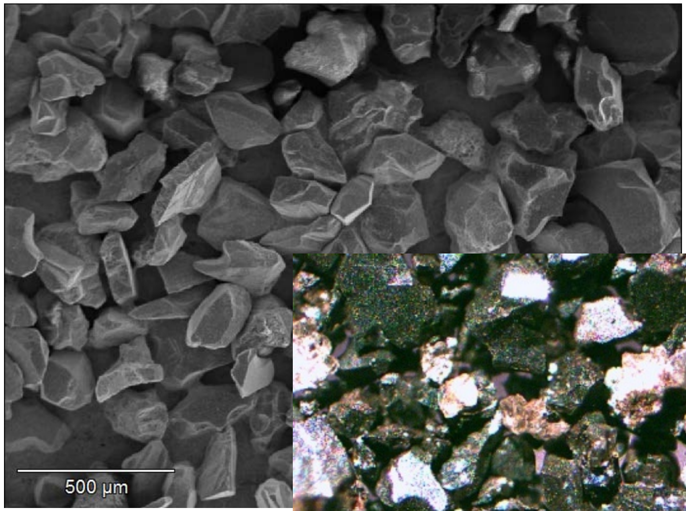
Configuration:

- Fuel Reactor – Bubbling Bed
- Air Reactor – Turbulent, transporting bed
- L-valve – to control solids circulation rate

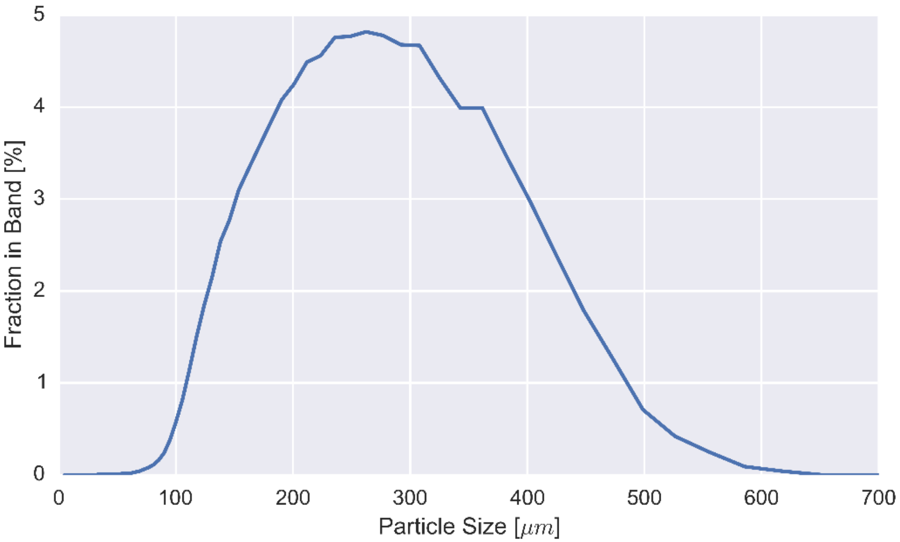


Oxygen Carrier Material: Raw Hematite

Material: Natural Hematite Ore
Source: Wabush Mine, Canada



SEM and light microscopy of Hematite



Particle density	4.9	g/cm^3
Sauter Mean Diam.	210	µm
D_{50}	238	µm
Sphericty	0.876	--
U_{mf}	8.55	cm/s

Test Objectives

- Calibrate CMU microwave sensor at different solid circulation rates
- Establish baseline carrier loss ($/$MW_{th}$-hr) for hematite
- Establish baseline fuel conversion for hematite
- Evaluate solid degradation as a function of circulation time, or exposure time in the process

Changes And System Modifications

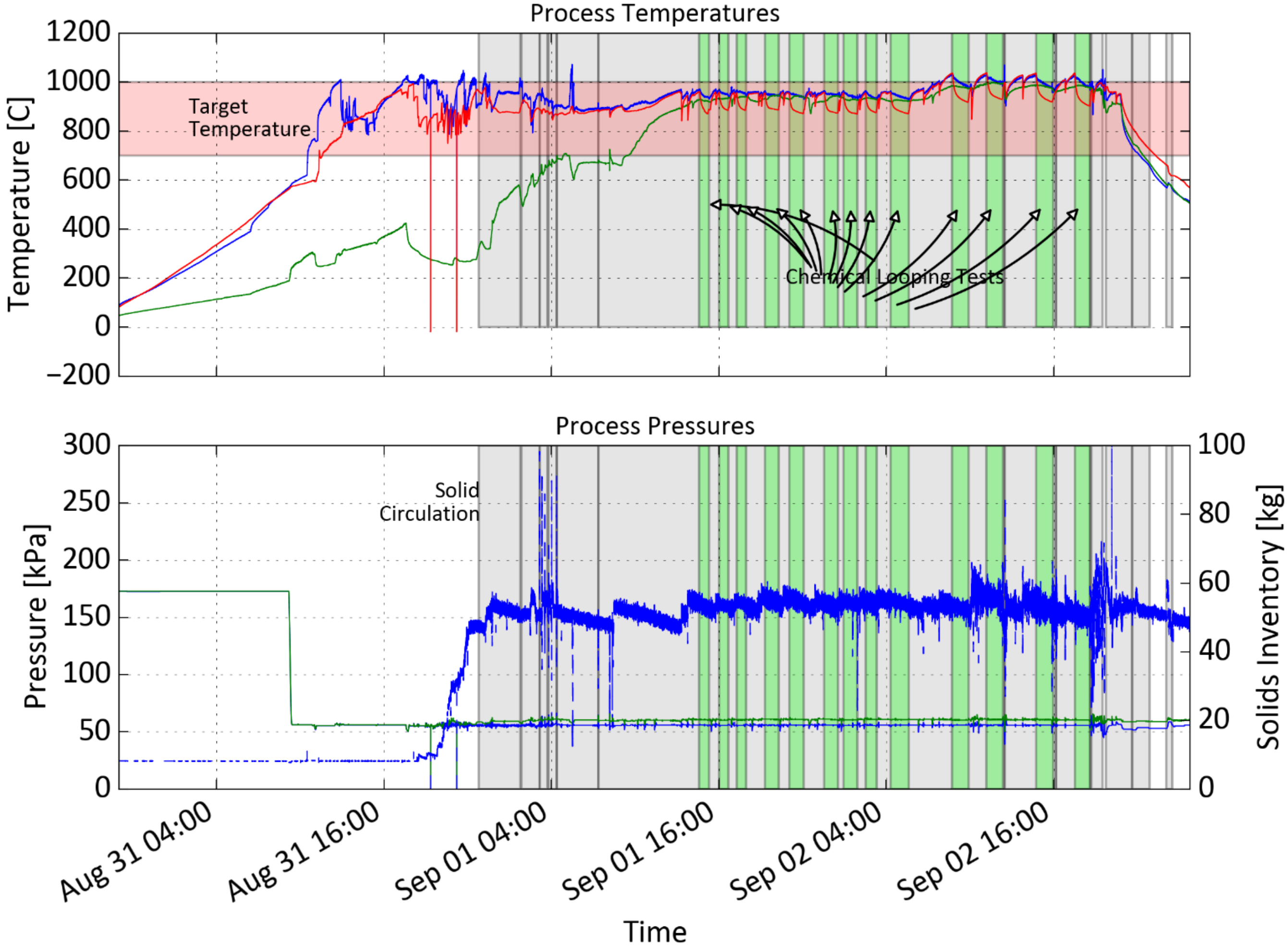
- New filters and filter housings for the fuel reactor and the cyclone vent lines
- Better insulation on fuel reactor vent lines
- Weigh scales on top-hat drains communicating with HMI and DAQ
- Fuel injection point control and recording
- New fuel reactor distributor plate design
- L-valve replaced and slight modifications to metal seal ring
- Two new condensate pots installed
- Volume added to top-hat drains for FR and LS
- Pressure controllers installed for gas analyzers
- Two new gas analyzers tested (borrowed from B13)
- Hematite carrier was pre-fluidized to remove fines

Test Log

- **Total Elapsed Time: 3 days 18 hrs**
- **Maximum Process Temperature: 1996.113 F**
- **Maximum Process Pressure: 17.36279 psi**
- **Total Circulation Time: 2 days 00:00:52**
- **Total Chemical Looping Time: 0 days 12:48:12**
- **Total Solids Added: 285.0 lbs**
- **Total Solids Drained From Top Hat: 125.68 lbs***
- **Solids Inventory at the end of test: 105.0521**

*This was the recorded value in the DAQ. Some additional fines were subsequently removed

Pressure, Temperature, and Inventory Summary



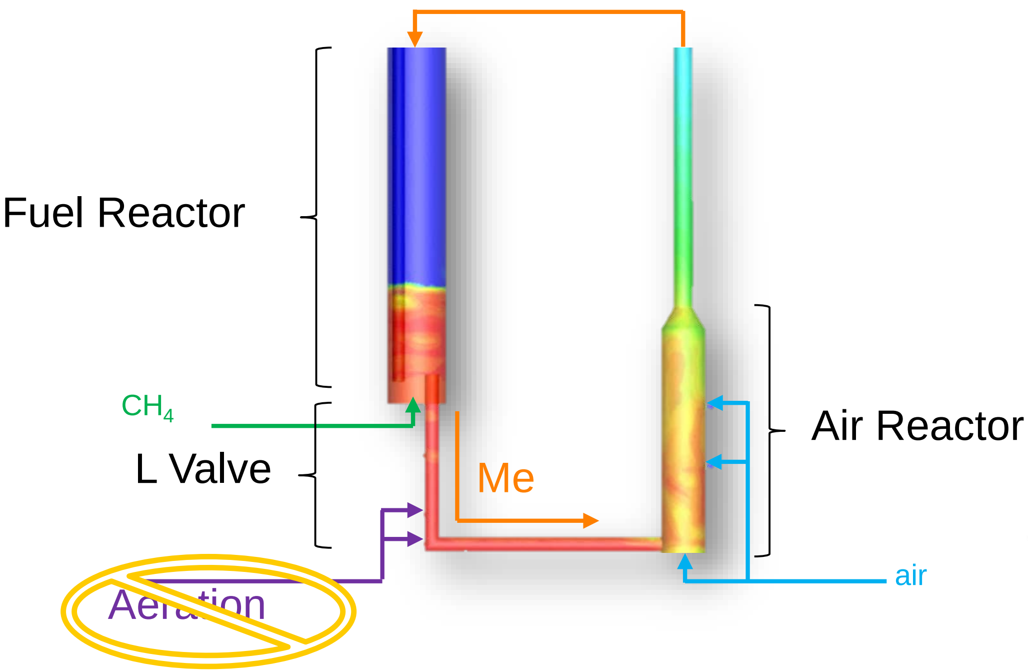
Circulation Rate: L-Valve Cut-Off

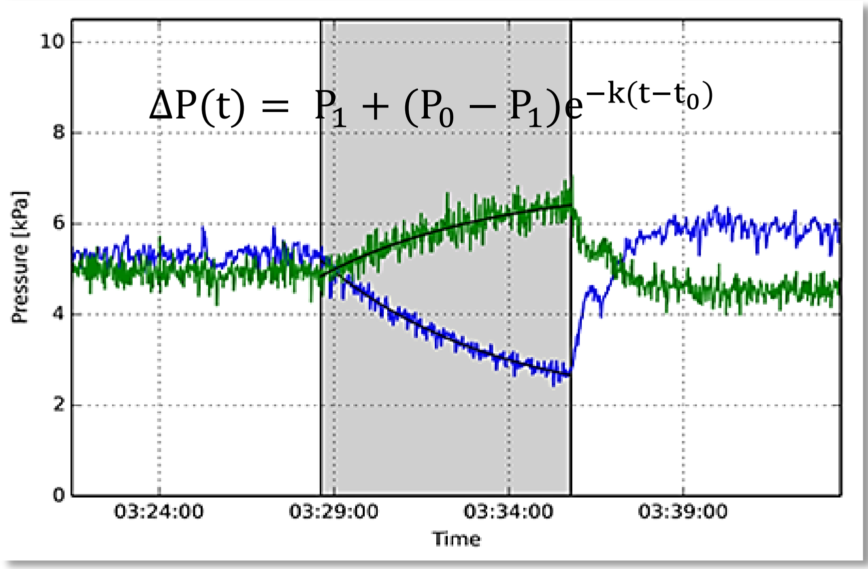
By breaking the loop, the circulation rate can be estimated assuming:

- L-valve stops flowing
- Bed pressure drop is related to the bed mass:

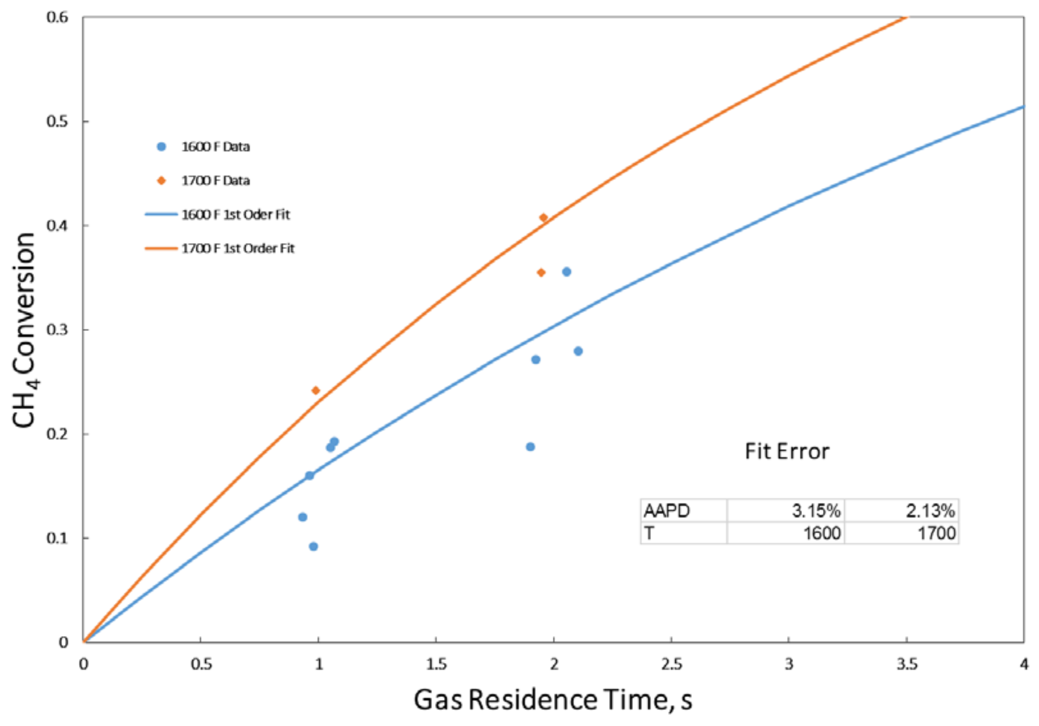
$$\Delta P = \frac{mg}{A}$$

$$\frac{dm}{dt} = \frac{A}{g} \cdot \frac{dP}{dt}$$





Fuel Conversion



- **Conversion fit to exponential decay**

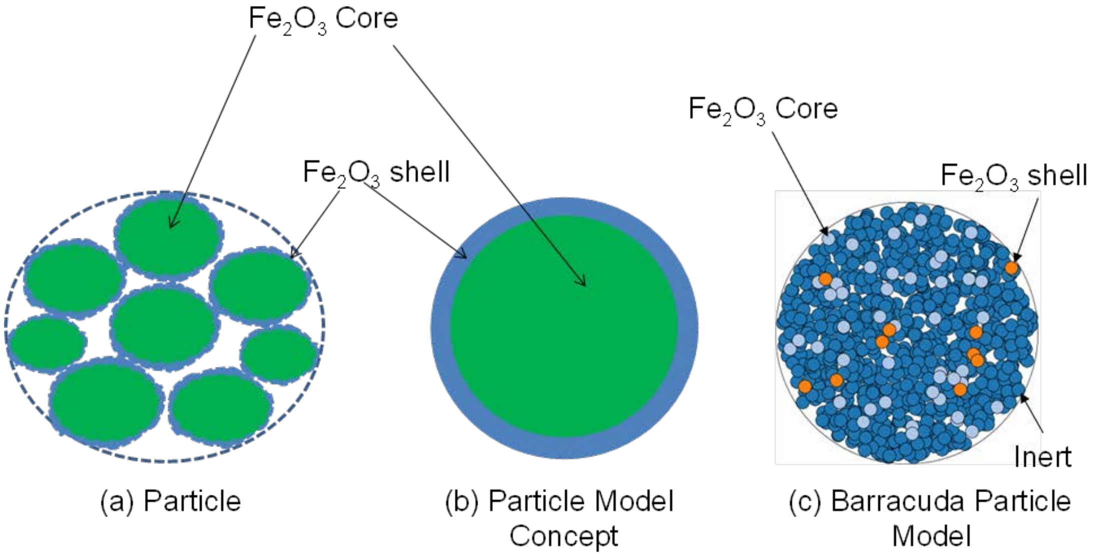
$$Conversion = 1 - e^{-\frac{t}{\tau}}$$

- **The AAPD was 3.15% for 1600 °F tests and 2.13% for the 1700 °F tests.**

Test Summary

- **Best run so far in terms of cumulative hours of CL operation**
- **No process upsets that resulted in significant solids carrier loss**
- **Solids mass closure improved, but further improvement is needed**
  - Most of discrepancy occurs during solids addition
  - Continue to investigate potential loss points
    - Flat bottoms on top-hat cyclones
    - Horizontal vent piping (particularly loop sent vent piping)
    - Condensate drains upstream of filters?
- **Data analysis needs to be completed**

Carrier Kinetics Cycle 1

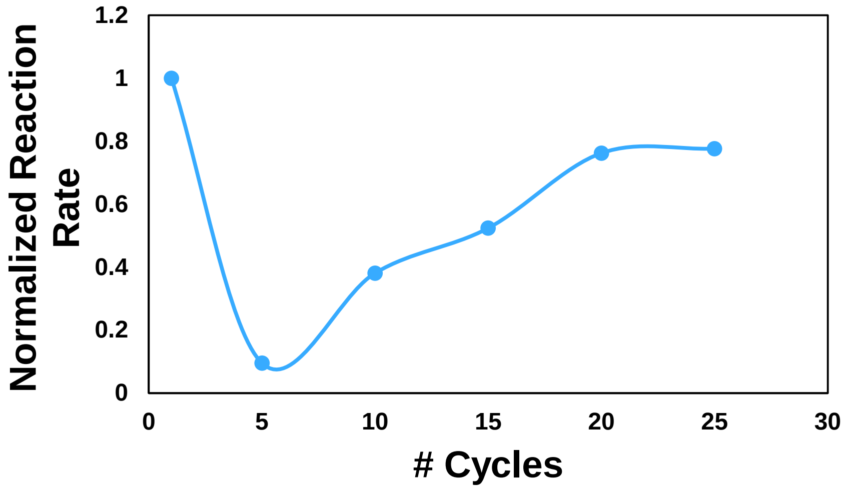


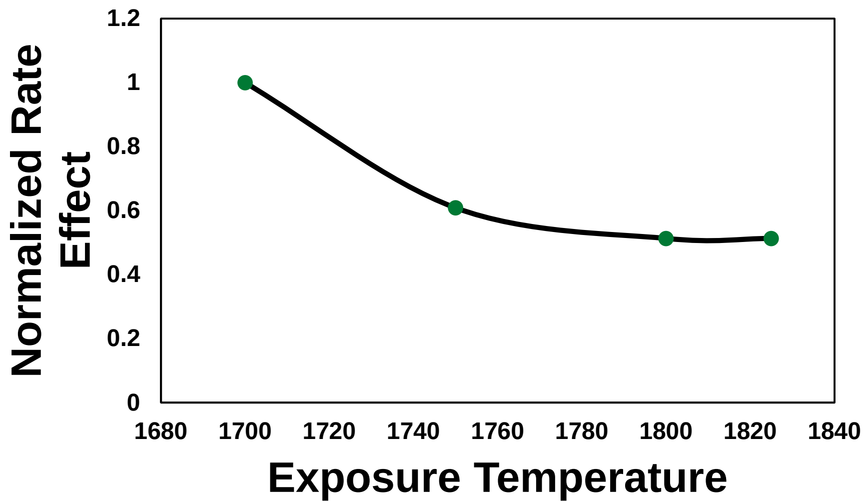
Barracuda model kinetic expression $$k = Ae^{\frac{-E}{RT}} m_i^b m_t^{(1-b)} \left(1 - \frac{m}{m_0}\right)_s^n \left(\frac{m}{m_0}\right)_c^m$$

Kinetic model parameters

Surface or Core	Species	A	E/R	b	n	m
Surface	CH_4	42000	16346	.667	NA	NA
Surface	CO	20	9707	.667	NA	NA
Surface	H_2	350	7818	.667	NA	NA
Core	CH_4	1400	16346	.667	1	1.333
Core	CO	40	9707	.667	1	1.333
Core	H_2	700	7818	.667	1	1.333

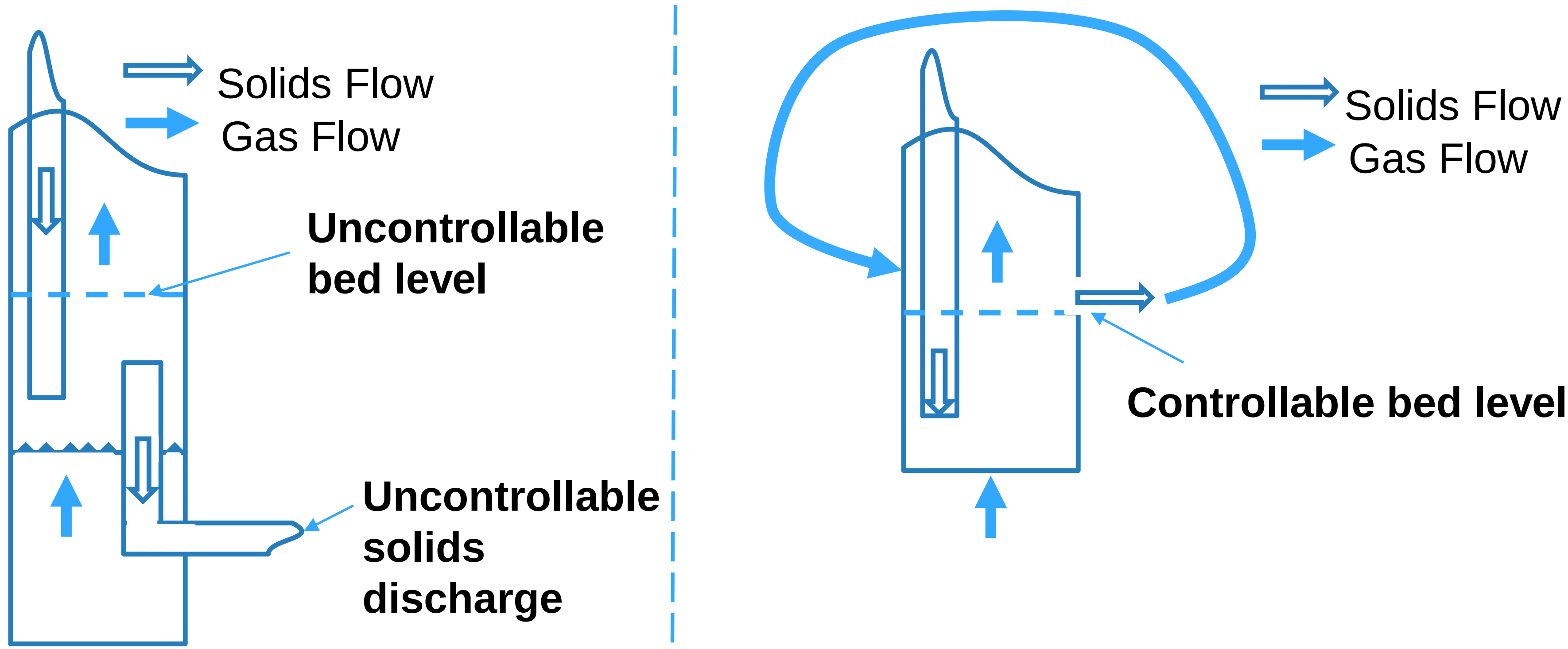
Adjustments to Kinetics –
Effects of Cycling and Exposure Temperature





Surface or Core	Species	A – Cycle 1	A - adjusted
Surface	CH_4	42000	563
Surface	CO	20	16
Surface	H_2	350	281
Core	CH_4	1400	16889
Core	CO	40	8
Core	H_2	700	141

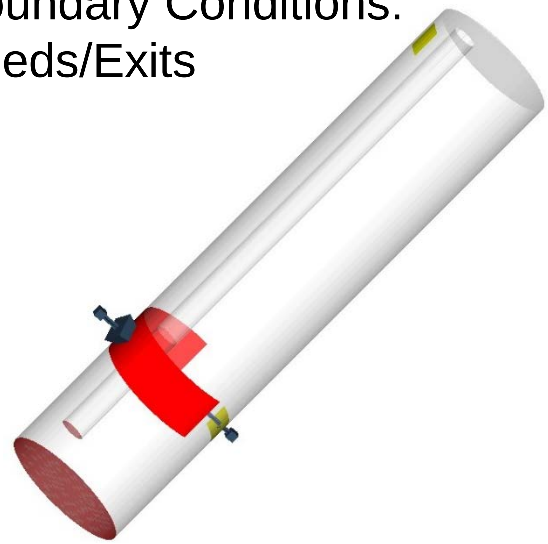
Barracuda Model Concept



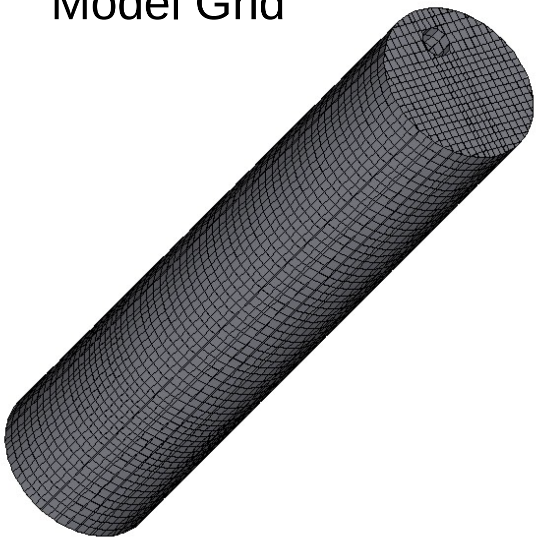
CLR Actual Configuration | **Barracuda Model Configuration**

Barracuda CFD Model

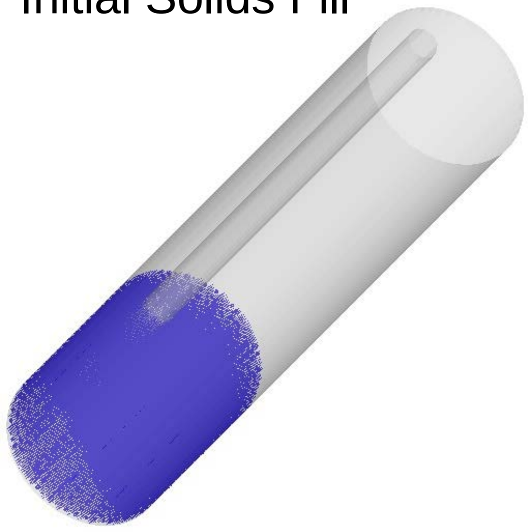
Boundary Conditions: Feeds/Exits



Model Grid

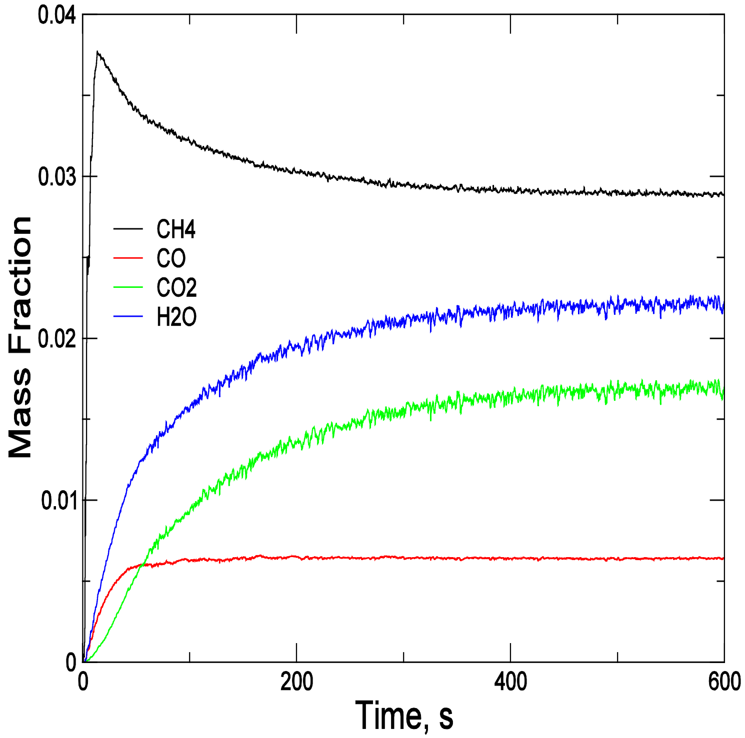


Initial Solids Fill

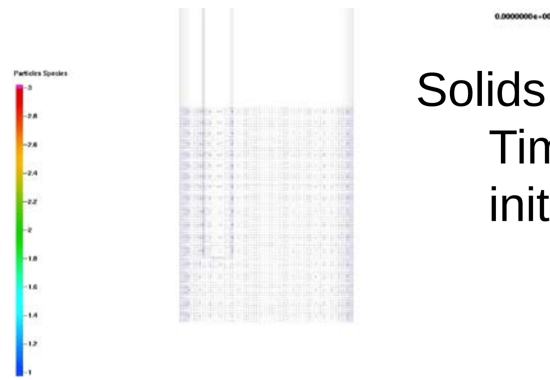


Model Parameter	Value
Cells	21524
Clouds	2.53e5
Particles	4.63e8
Mass	1.5kg

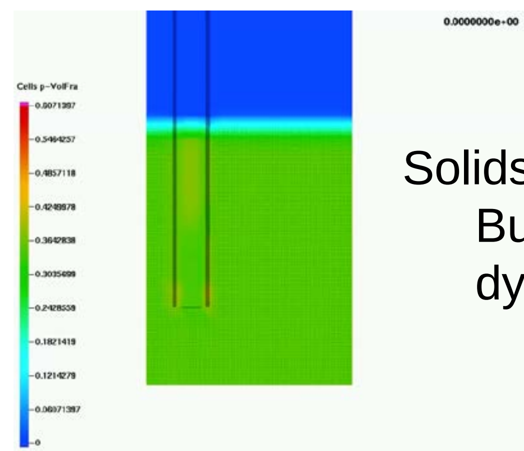
Barracuda Simulation



- **Solids residence time is about 210 second**
- **600 seconds needed to effectively stabilize the concentration – this provides 87% replacement of initial charge vs 95% expected for fully mixed.**
- **Bubbles near standpipe – likely carrying some fresh feed to top of bed which escapes in this configuration.**

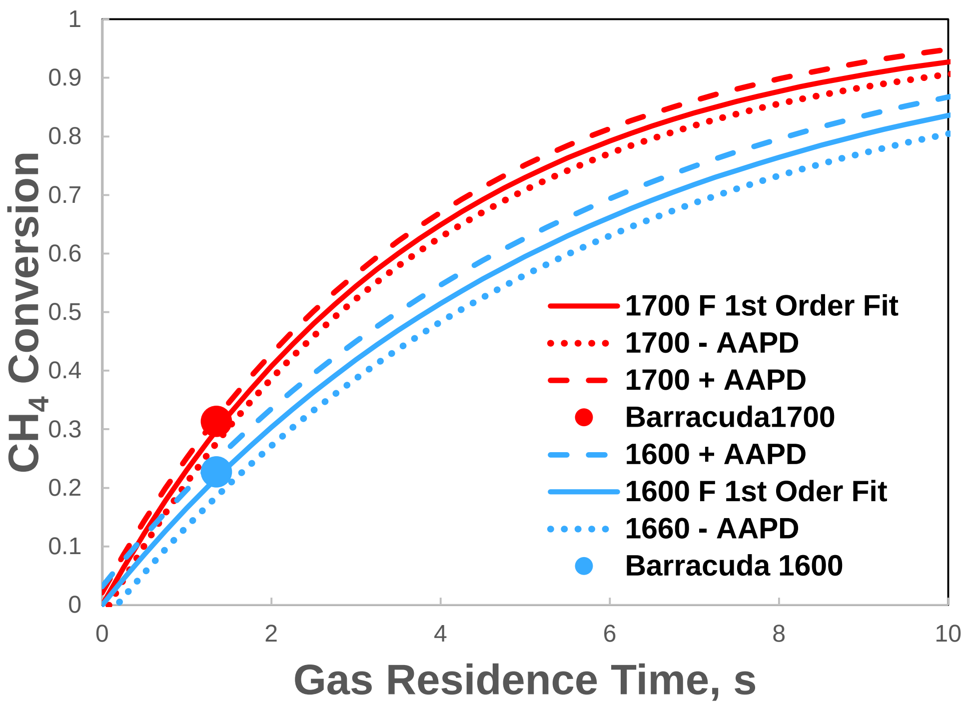


Solids Species – Time to purge initial charge



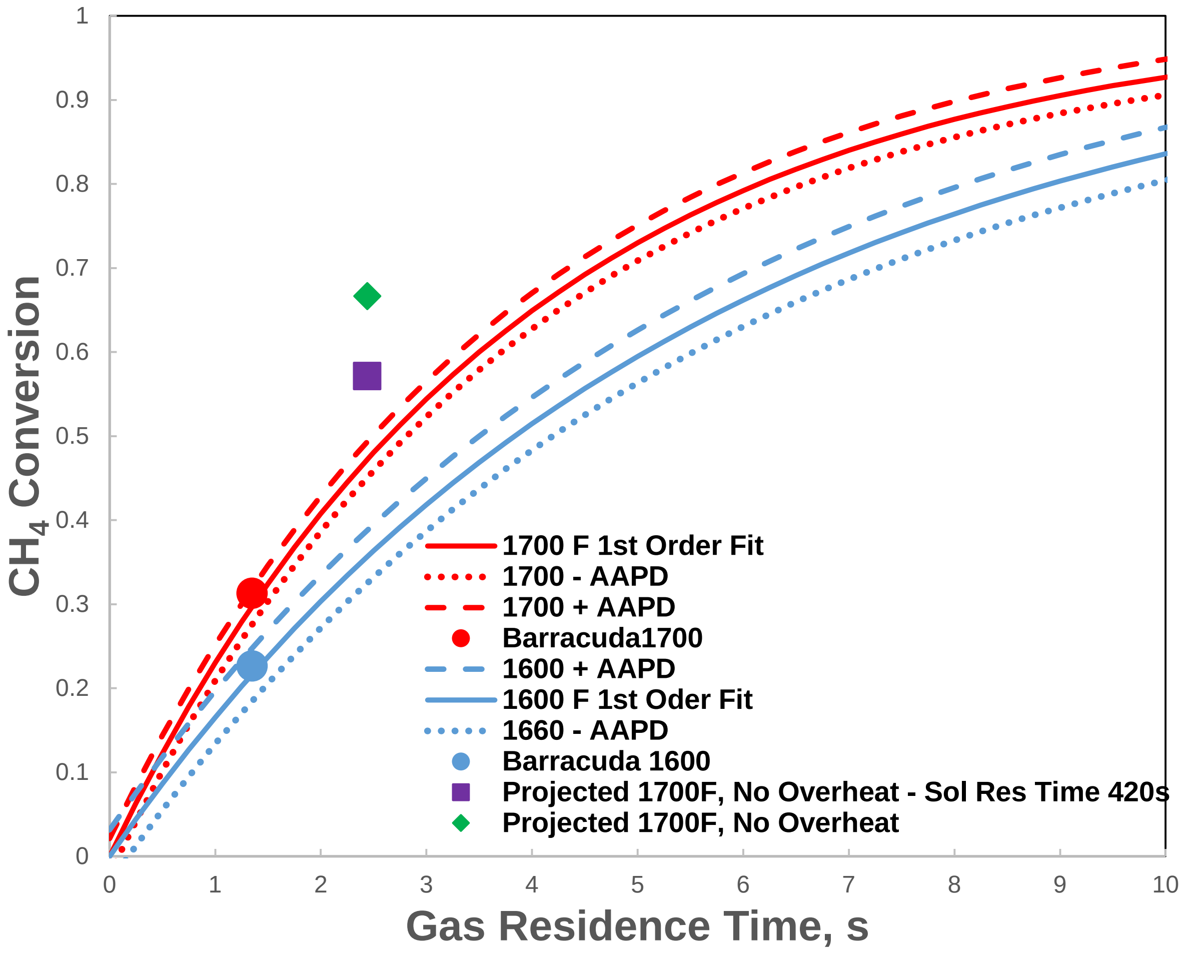
Solids Fraction – Bubble dynamics

Model Validation

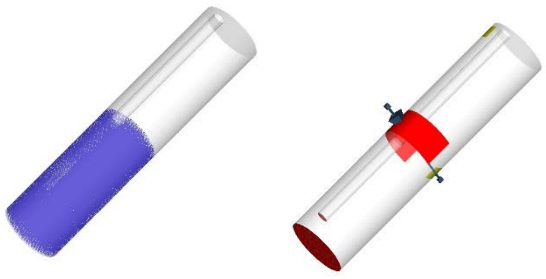


- **Two simulations run**
- **Error much less that the experimental variance as defined by the AAPD.**
- **Model Validated.**
- **Question**
  - What will it take to get the CH4 conversion greater than 60%

Projected CH_4 Conversion - Solids Res. Time of 210 s.



Deeper Bed



- 67% Conversion for Case with 210 s and deeper bed
- Increasing the solids residence time decreases projected conversion – average kinetics of solids are lower.

Summary

- Barracuda model of fuel reactor successfully validated with error between model and experiment about 2%.
- Validated Barracuda model applied to future test conditions to predict conversion greater than 65%.
- Approximately 3 solids residence times are required to purge out the initial bed

Disclaimer

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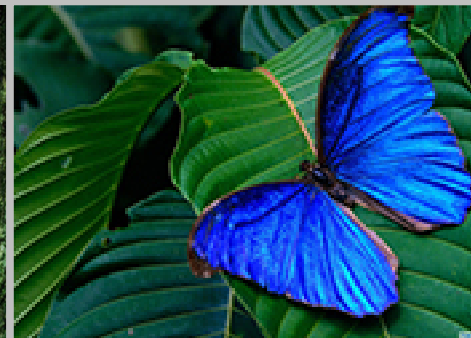
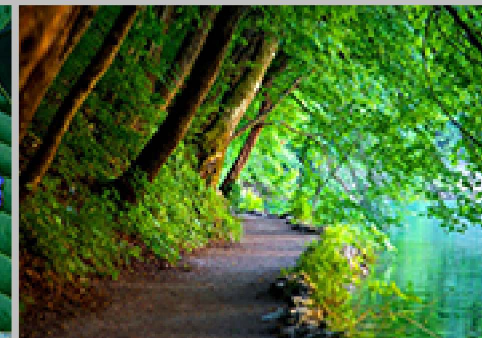

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QUESTIONS