

REMS Toolset



Framework for Optimization and Analysis

March 20, 2017 Gasification Systems Project Review, Dirk Van Essendelft

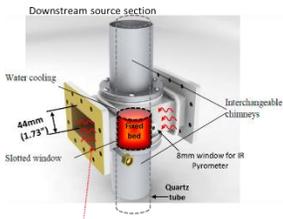
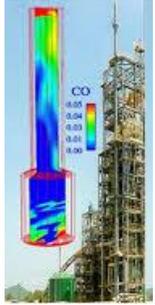


Solutions for Today | Options for Tomorrow



Advanced Reaction Systems

Project Overview



Task 1: Project Management

Task 2: Microbial Enhanced Coalbed Systems (MECS)

Task 3: Process and Reaction Intensification

- Microwave enhanced reaction systems
- Non-traditional thermal systems
- Enabling materials
- Oxygen carrier development for chemical looping gasification

Task 4: Virtual Reactor Design, Validation, and Optimization

- Basic MFiX code development
- Test system validation with physical experiments
- Optimization toolsets

Task 5: Systems Engineering and Analysis

- Feasibility and baseline study
- Metric development
- Pathway studies

MFS REMS Team



Software

K. Buchheit

T. Jordan

T. Li

D. Van Essendelft

J. Weber

Experimental

G. Breault

B. Gopalan

W. Rogers

J. Tucker

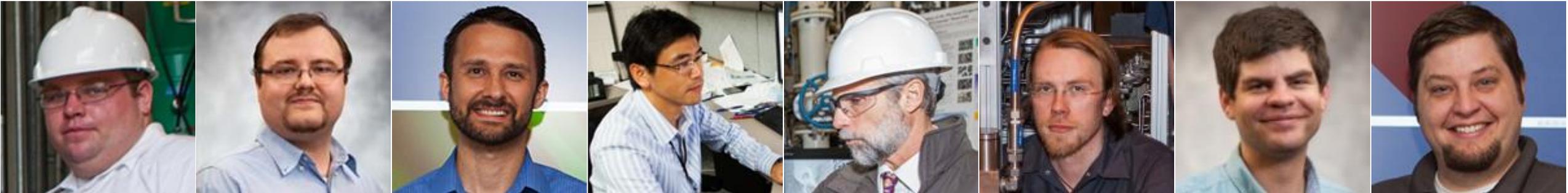
Management

J. Fisher (EPAT)

C. Guenther (MFS TL)

W. Rogers (FWP TTC)

M. Syamlal (SF)



What is Optimization?

The REMS Toolset



“[An] act, process, or methodology of making something (as a design, system, or decision) as fully perfect, functional, or effective as possible.”

<http://www.merriam-webster.com/dictionary/optimization>

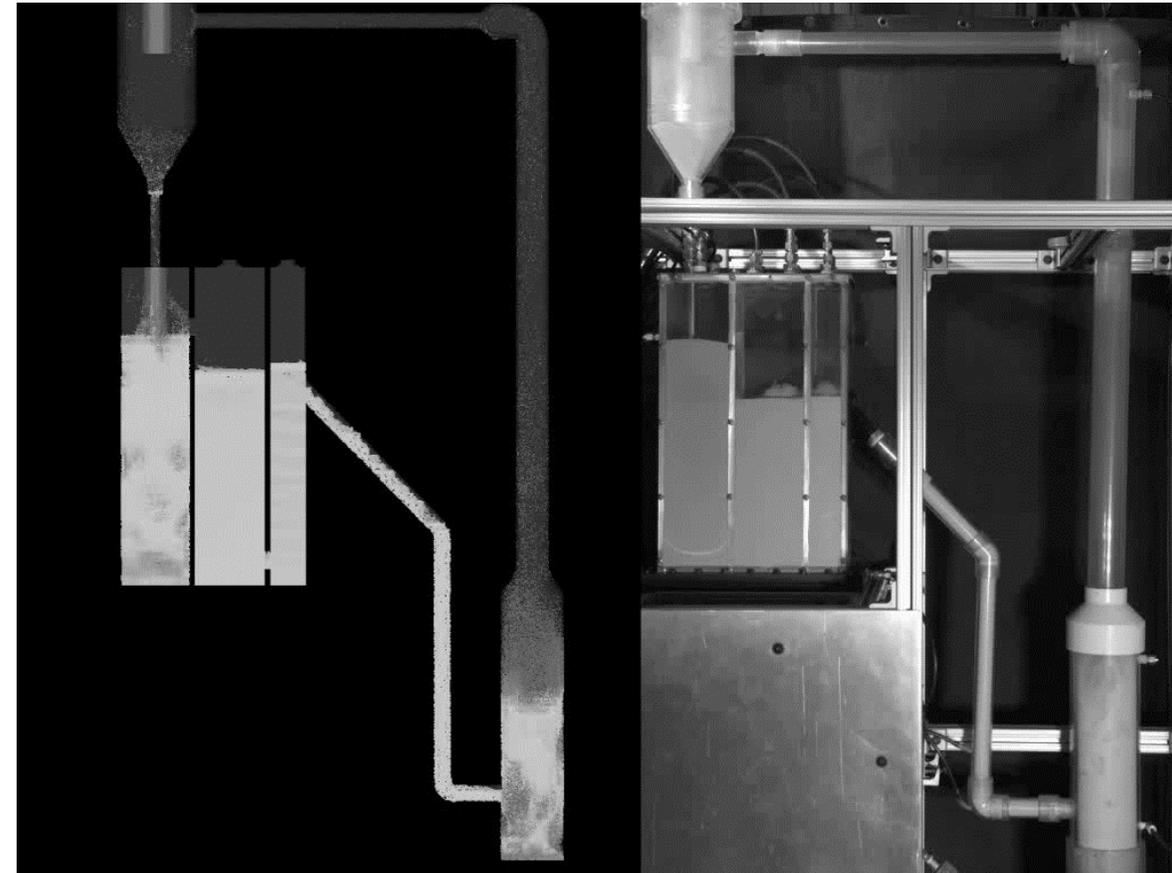
“[A] mathematical technique for finding a maximum or minimum value of a function of several variables subject to a set of constraints, as linear programming or systems analysis.”

<http://www.dictionary.com/browse/optimization>

The Goal: CFD Based Optimization

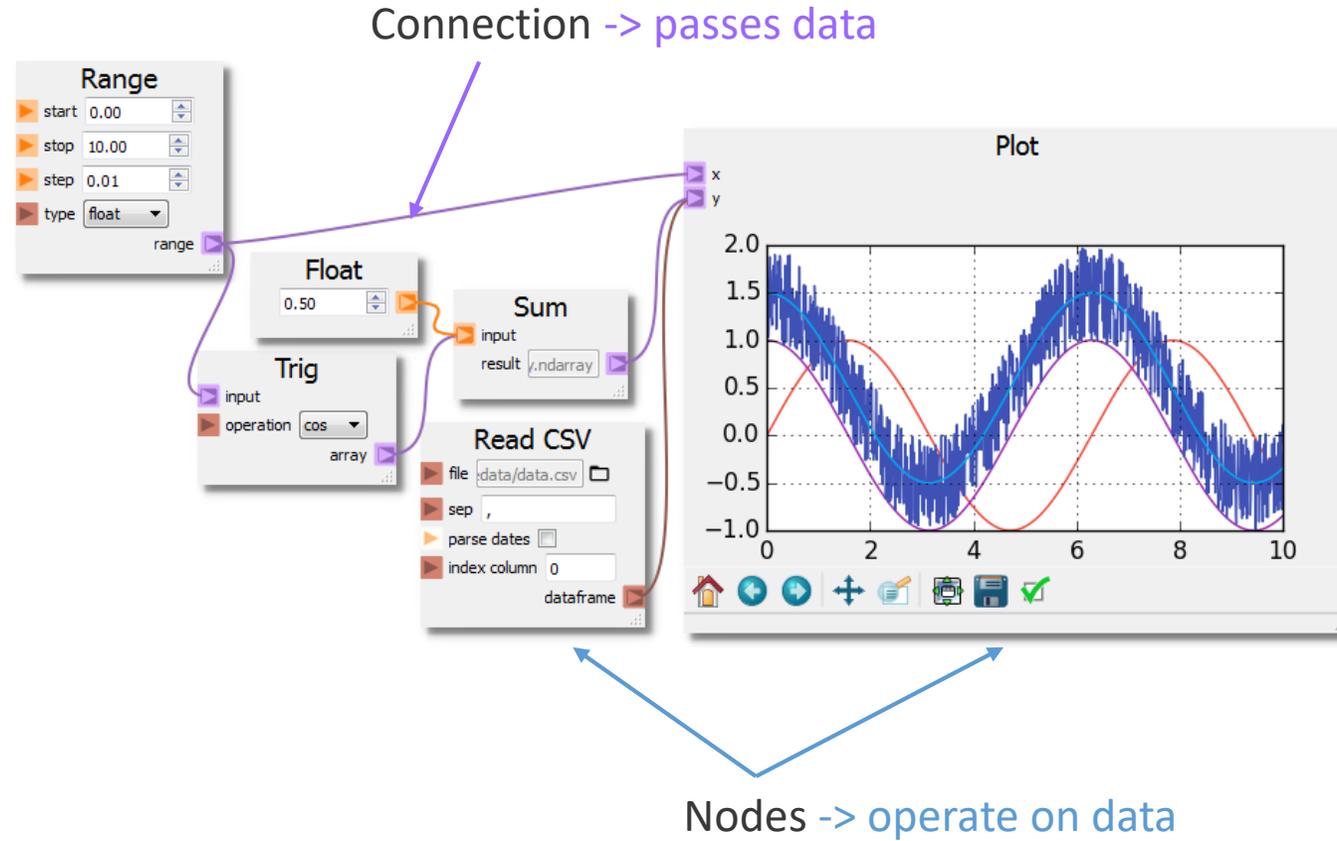
The REMS Toolset

- Computational Fluid Dynamics (CFD) provides:
 - Quick, Inexpensive way to investigate a design
 - Unique physical insight into complex processes
 - Quantitative information
- We want leverage our expertise in CFD and the quantitative information it provides to optimize real systems
- Our *Optimization Toolset* is needed to allow practitioners to scan through a large number of variations to determine the optimal design parameters quickly and efficiently
 - Based on NETL's PyQtNode software
 - Integrated into NETL's **MFiX Suite** of multiphase CFD software for predicting reactor performance
 - Already being applied to guide real world optimal designs



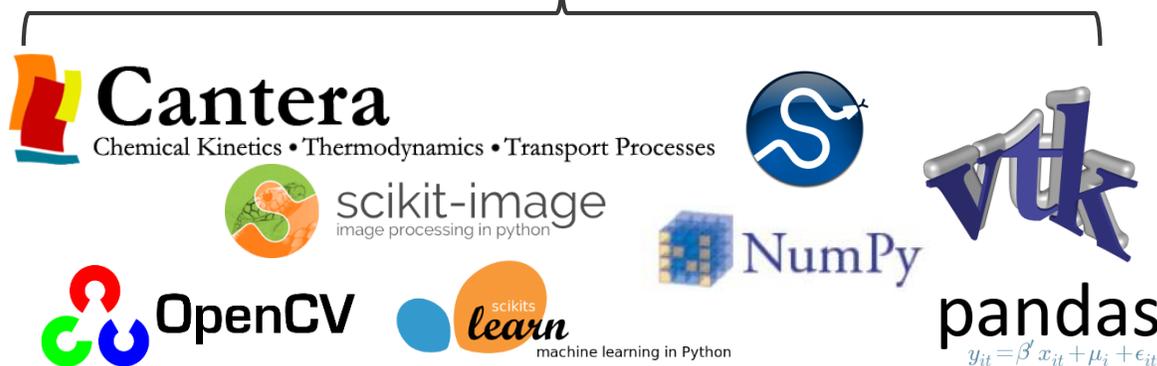
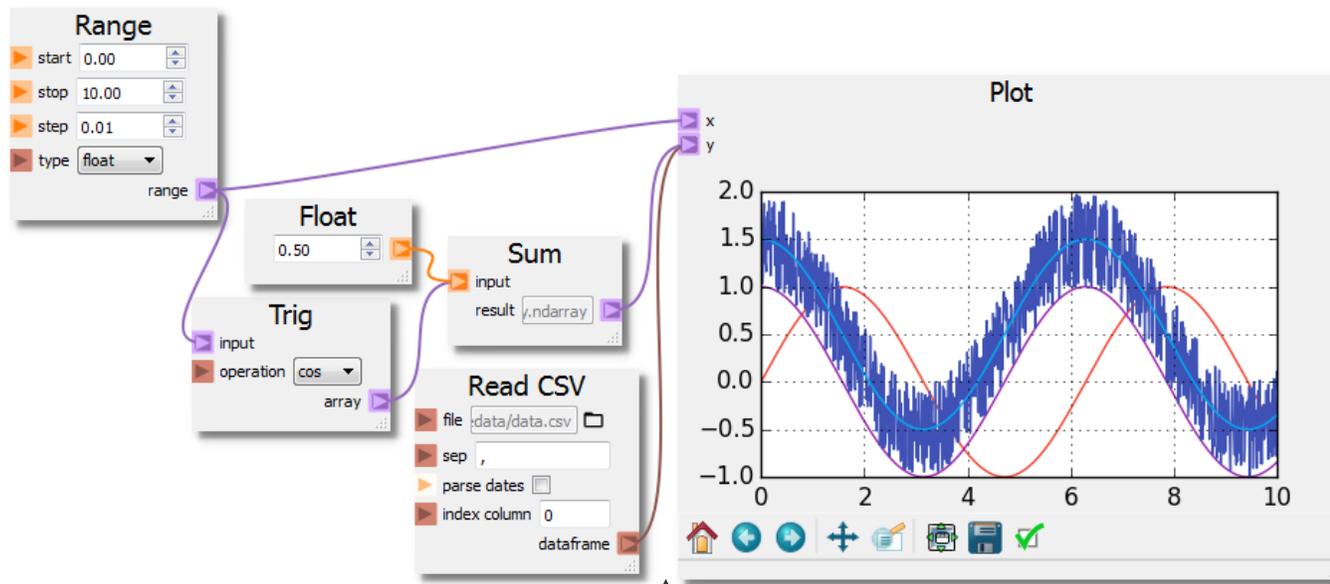
What is pyqtnode?

Graphical Programming Library



What is pyqtnode?

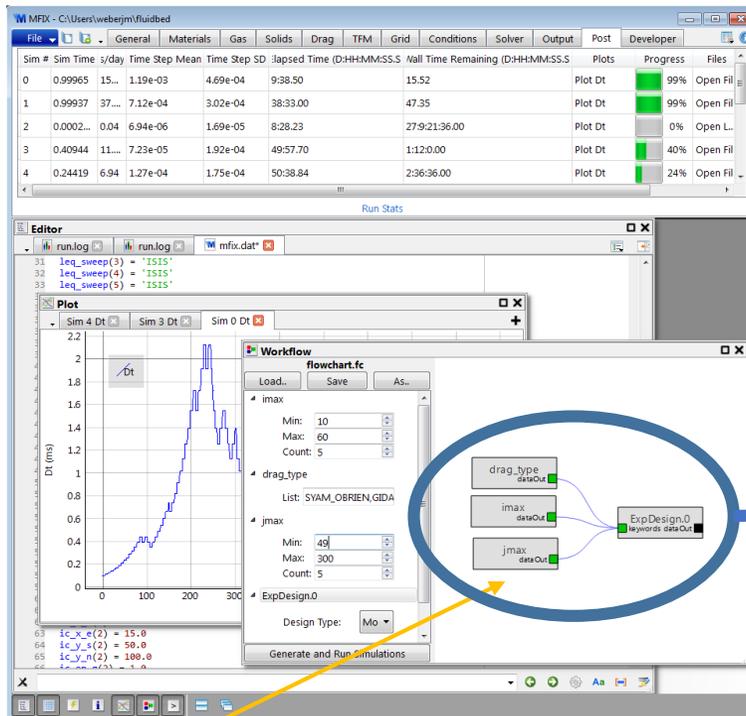
Graphical Programming Library



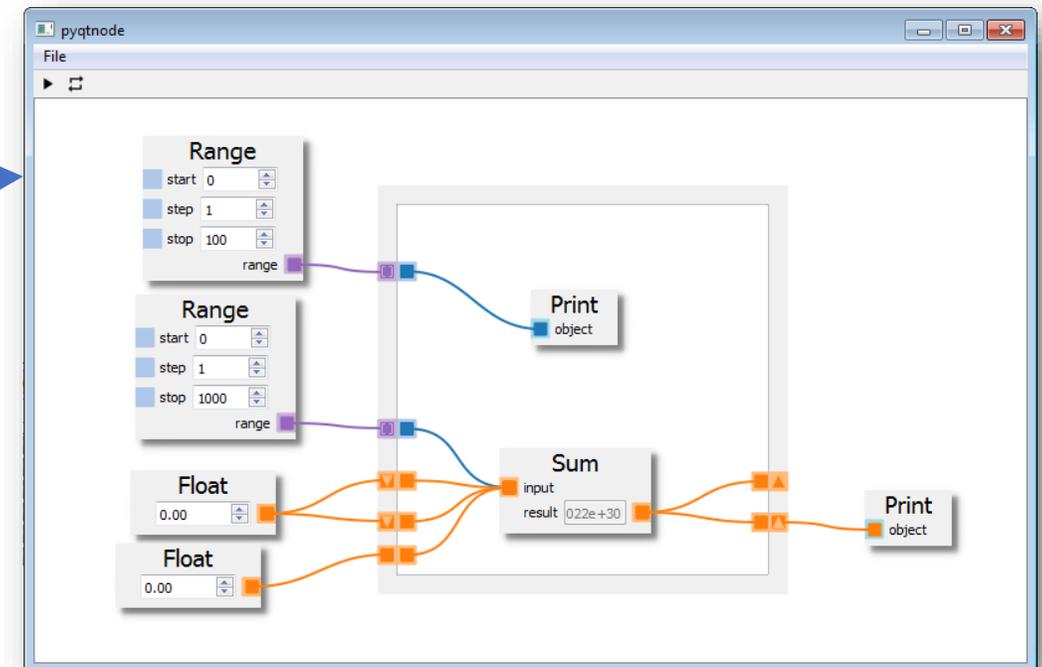
Where did PyQtNode start?

Graphical Programming Library

First DOE run with MFX from the MFX-GUI
Carol Sadek, MLEF Summer 2015
Mentor: Justin Weber



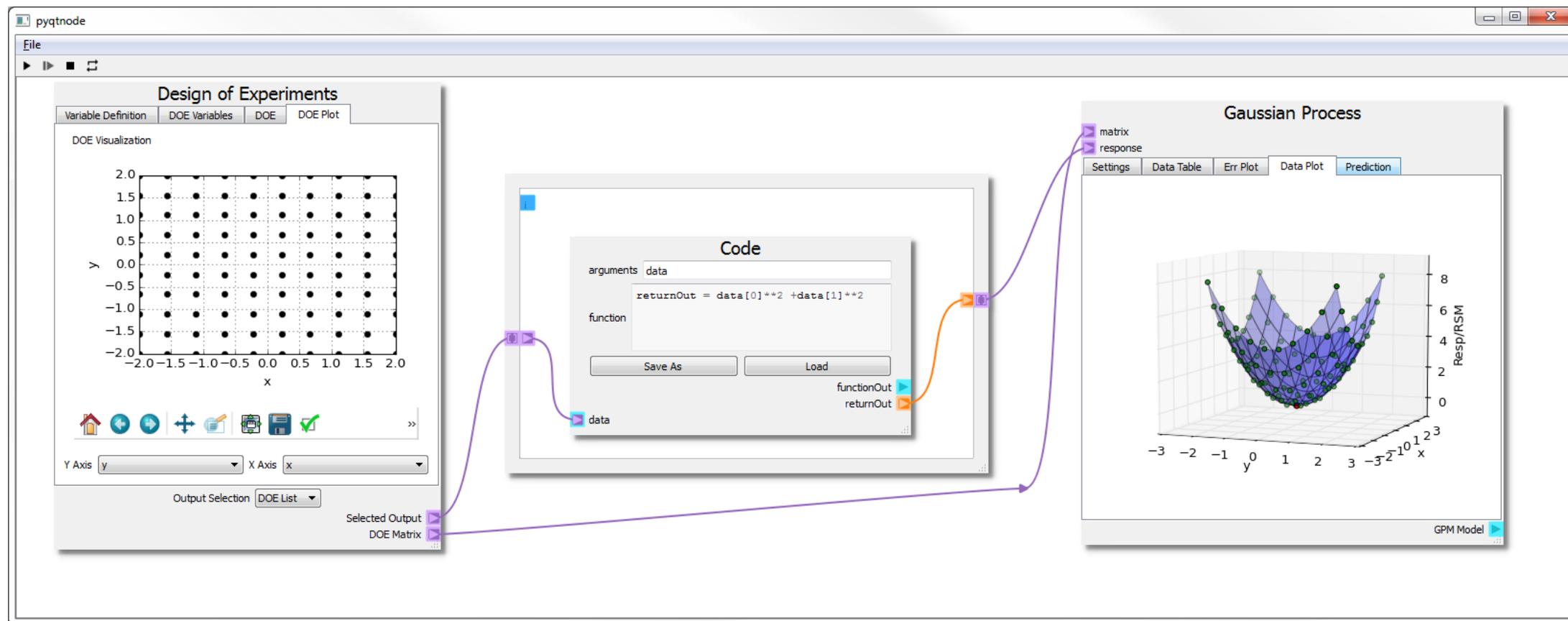
Justin Weber's start in PyQtNode



Pyqtgraph
(opensource python library)

Find the Bottom of a Bowl

The REMS Toolset: Minimize $f(x, y) = x^2 + y^2$



Integrated CFD Optimization

The REMS Toolset: MFIx and the MFIx GUI



Name	Model	Diameter	Density
Solid 1	DEM	8.0000e-04	1.1300e+03

Options:

- Solve U-Momentum Equation
- Solve V-Momentum Equation
- Solve W-Momentum Equation
- Enable Species Equations
- Enable Scalar Equations

Parameters:

- Diameter: 8.0000e-04 m
- Density: Constant 1.1300e+03 kg/m³
- Viscosity: Continuum Solids Pa
- Mol. weight: Mixture kmol/kg
- Spec. heat: Mixture kJ/(kg K)
- Therm. cond.: Constant W/(m K)
- Emissivity:

Species:

```
kn = 1.0000e+03
bc_z_t(1) = 0.105
bc_z_t(2) = 0.095
cartesian_grid = True
nlog = 5000
bc_x_e(1) = 0.31
```

Design of Experiments

DOE Visualization

Y Axis: imax, X Axis: jmax

Output Selection: Complete

Selected Output: DOE Matrix

```
Welcome to MFIx - https://mfix.netl.doe.gov
MFIx-GUI version 0.2y
Loading MINI-CFB.mfx from N:/mfix/benchmarks/dem/mini-cfb
Solver: MFIx-DEM
Loaded MINI-CFB.mfx
```

Optimization Using MFIx

The REMS Toolset

2:1 Particle Density Ratio
4:3 Diameter Ratio

Rectangular Bed

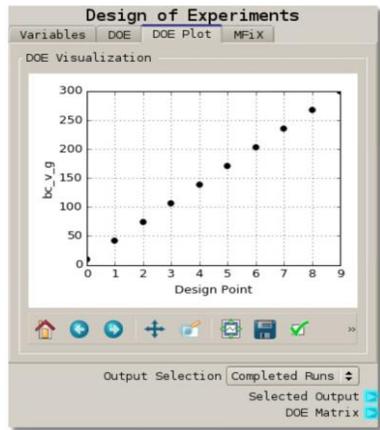
Particles Randomly placed in initial state

Uniform gas velocity

Gas Velocity Too Low - Under Fluidized

Optimal Gas Velocity

Gas Velocity Too High - Over Fluidized



Shell Run

working directory Does Not Exist

Shell Command `grep Time_SEG_DES.pvd > tt2.txt`

Path Join

path1 `/rems/runs/test_000009`

path2 `tt2.txt`

output `s/test_000009/tt2.txt`

loadtxt

file Does Not Exist

skiprows 0

usecols 1,4,5,8,9

array

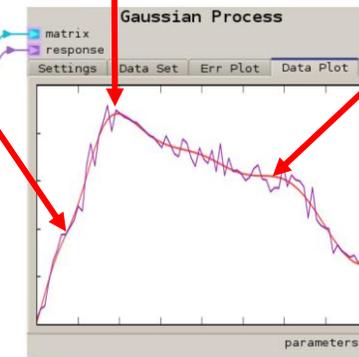
Code

```
arguments data, gasVelocity
import numpy as np
start_time = 2.05
resid_cutoff = 10000
start_search_frac = 0.3
plot = False
function
if plot:
import matplotlib.pyplot as plt
time = data[:,0]
lB = data[:,1]
lT = data[:,2]
hB = data[:,3]
hT = data[:,4]
mask = np.where(time >= start_time)
```

Save As Load

functionOut
returnOut

data
gasVelocity



Maximize

function
initialGuess
result

Print

tag optimalVel
object

List

0 100
+ -
list

Build a DOE & Run MFIx

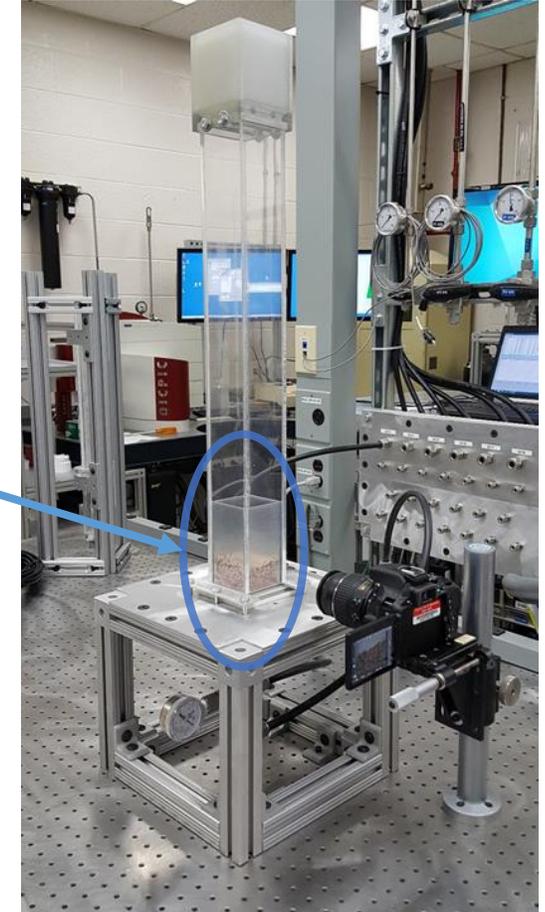
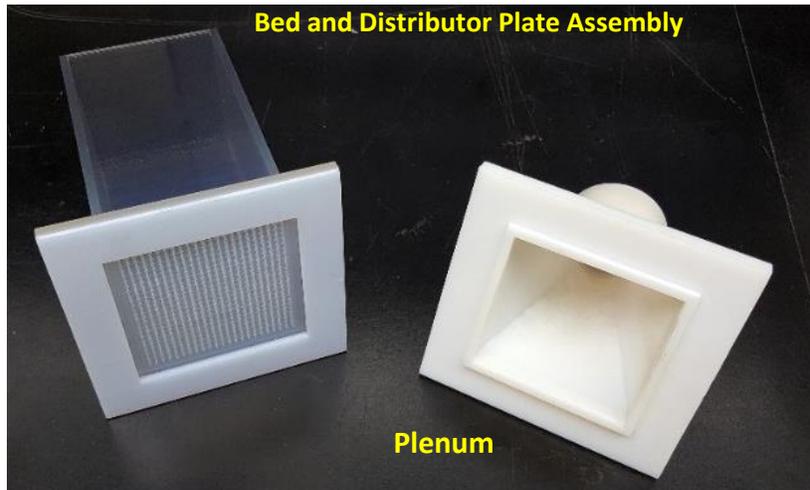
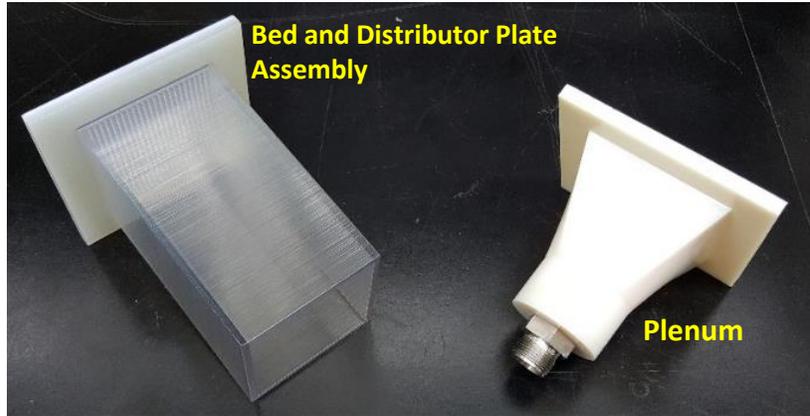
Process and Analyze Data

Build Surrogate

Optimize

3D Print Geometry

REMS Toolset: Validation



Experimental Validation

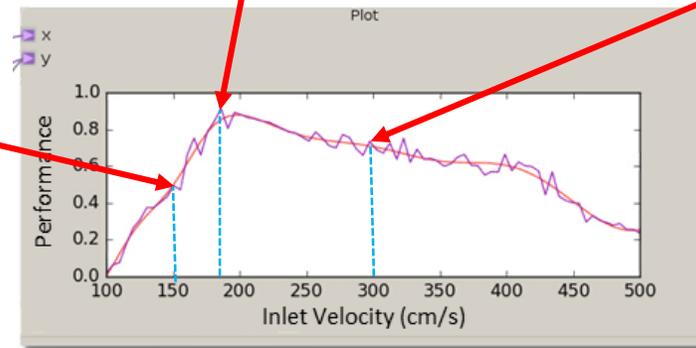
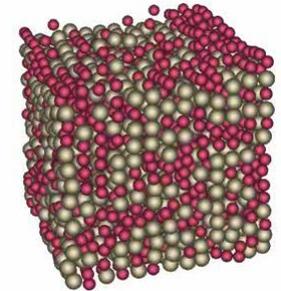
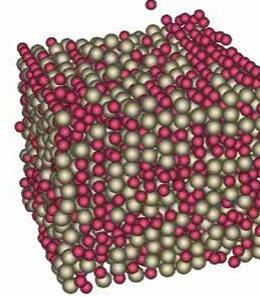
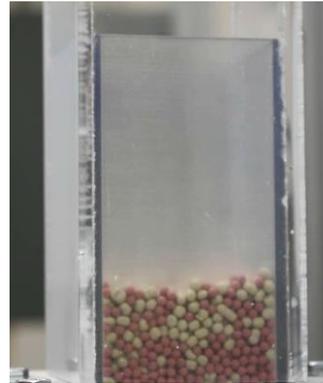
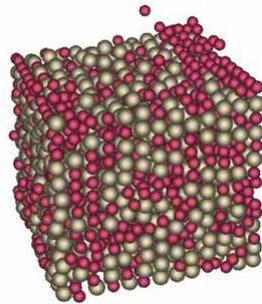
The REMS Toolset: Validation

An image analysis-based technique being developed for quantitative comparison

Optimal Gas Velocity

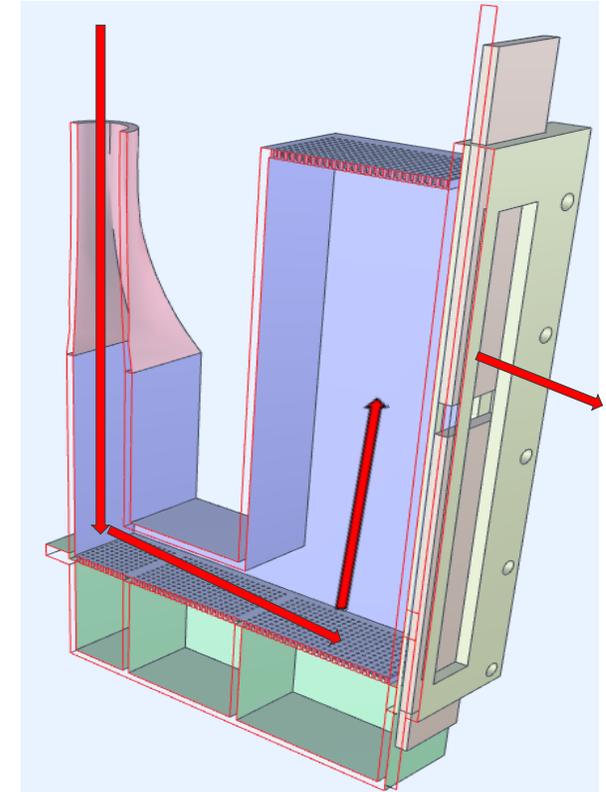
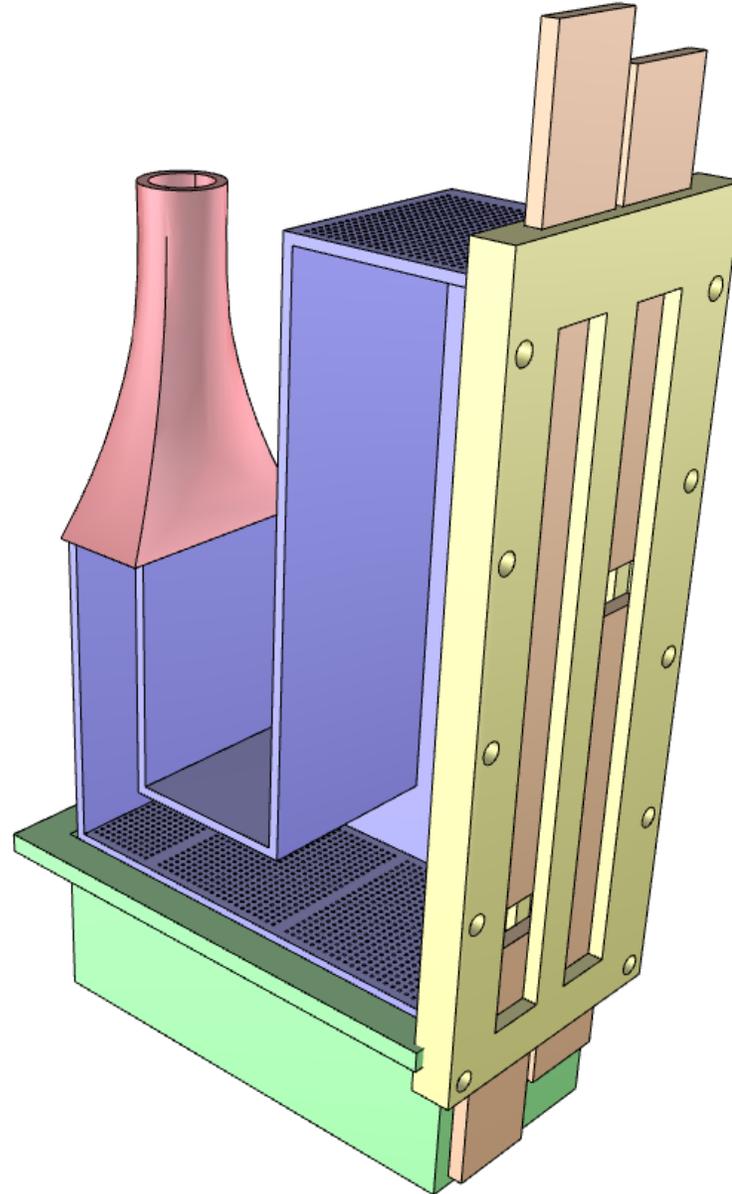
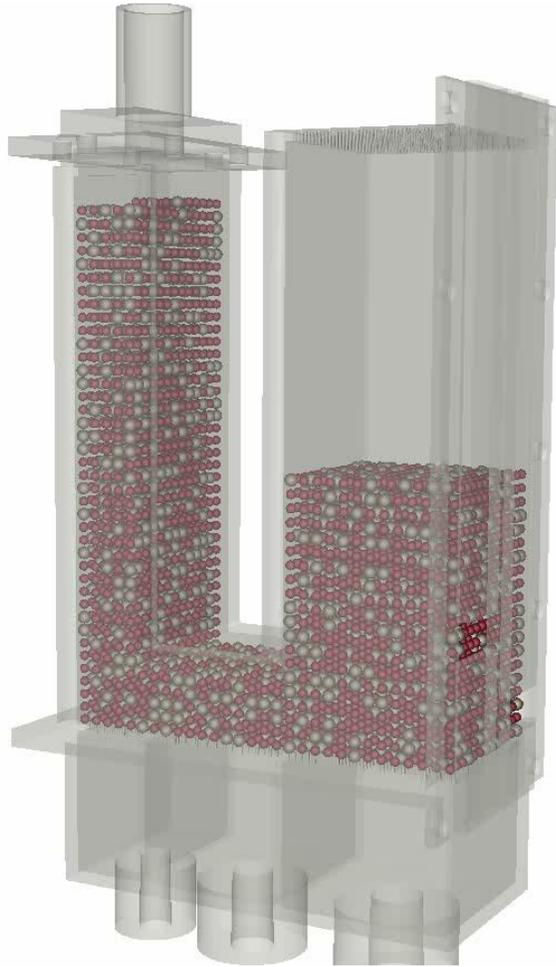
Gas Velocity Too Low - Under Fluidized

Gas Velocity Too High - Over Fluidized



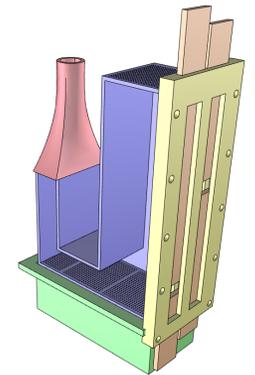
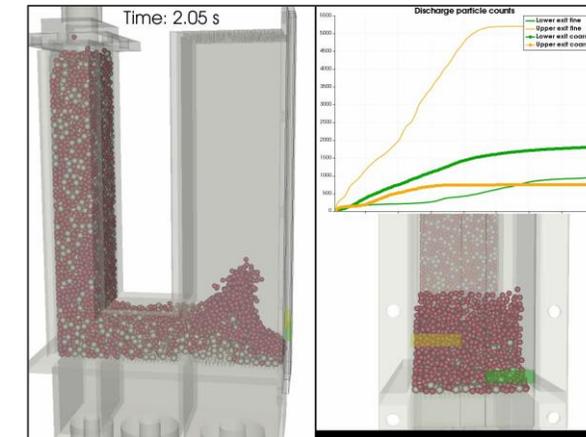
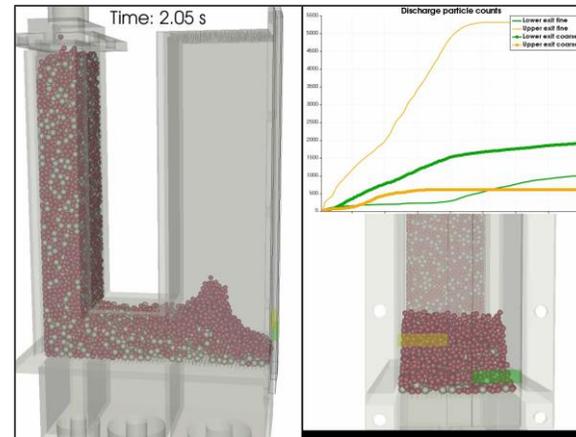
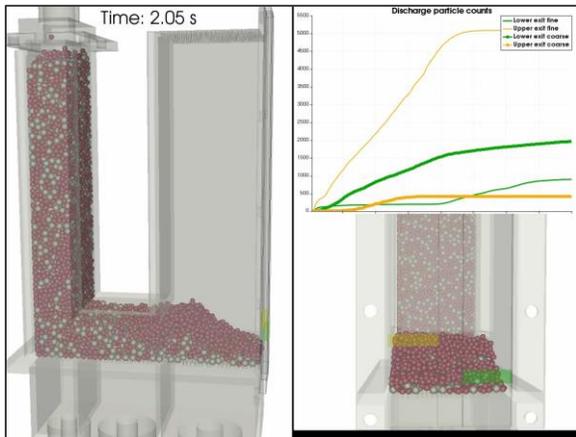
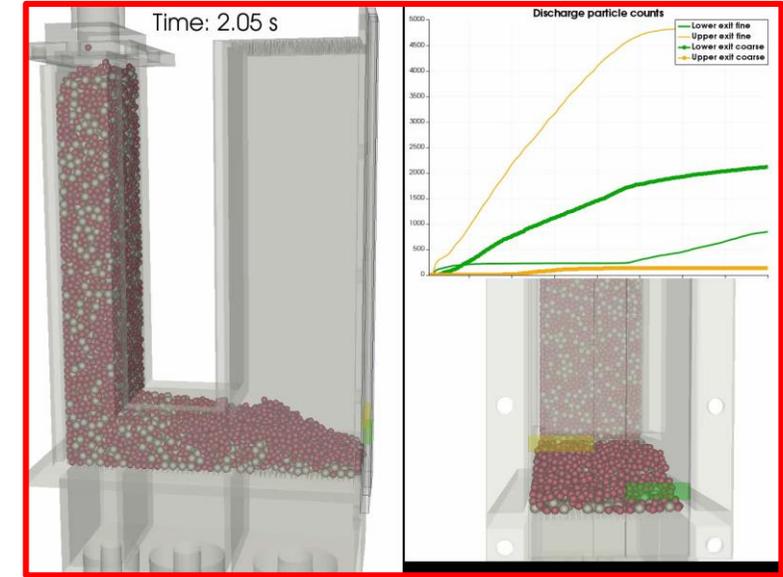
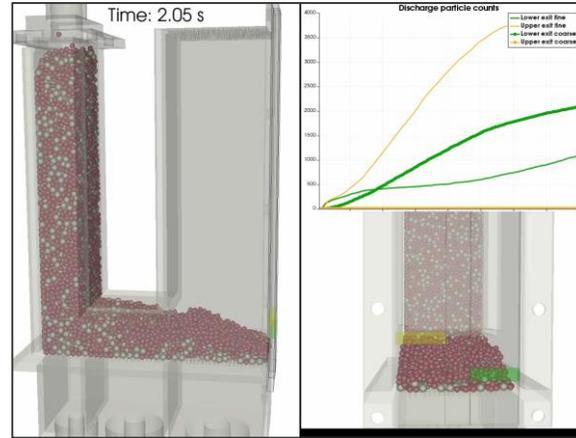
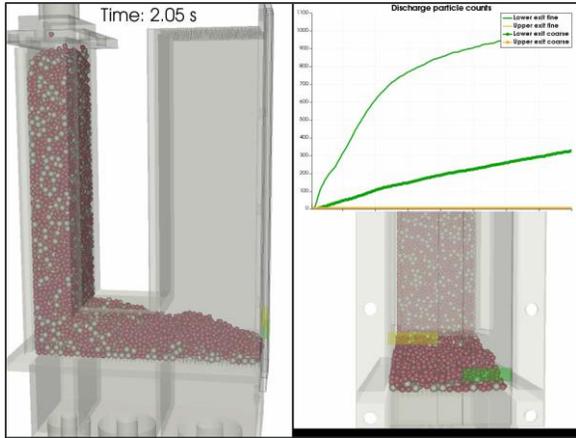
Continuous Flow

The REMS Toolset: Stepping it up!



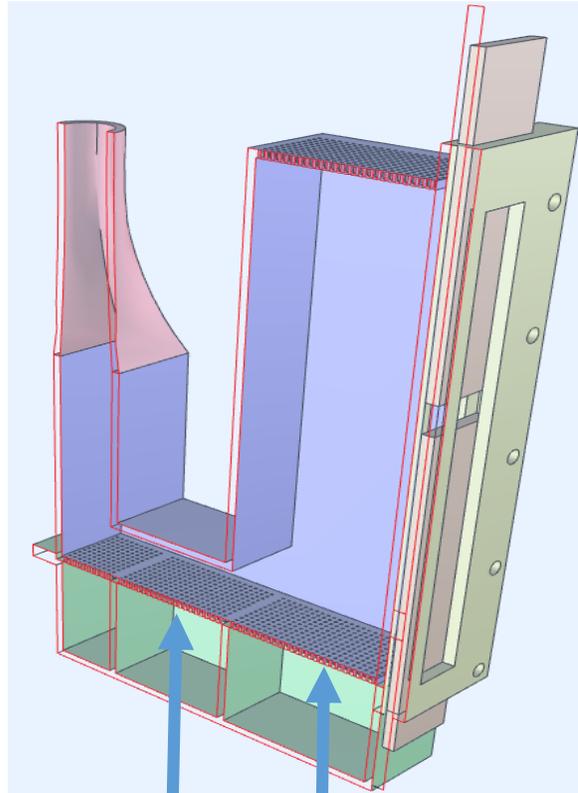
Continuous Flow

The REMS Toolset: Parametric Study of Flow Control



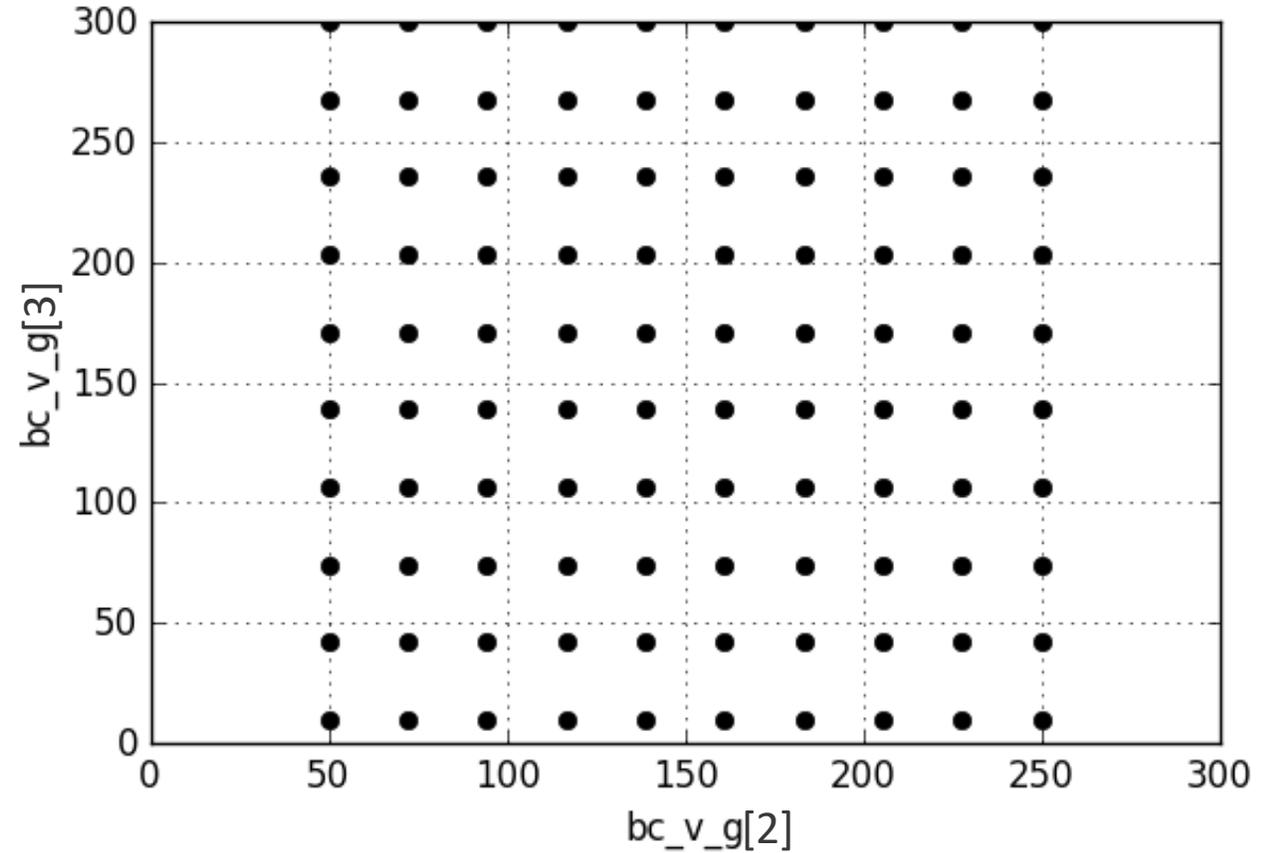
Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization



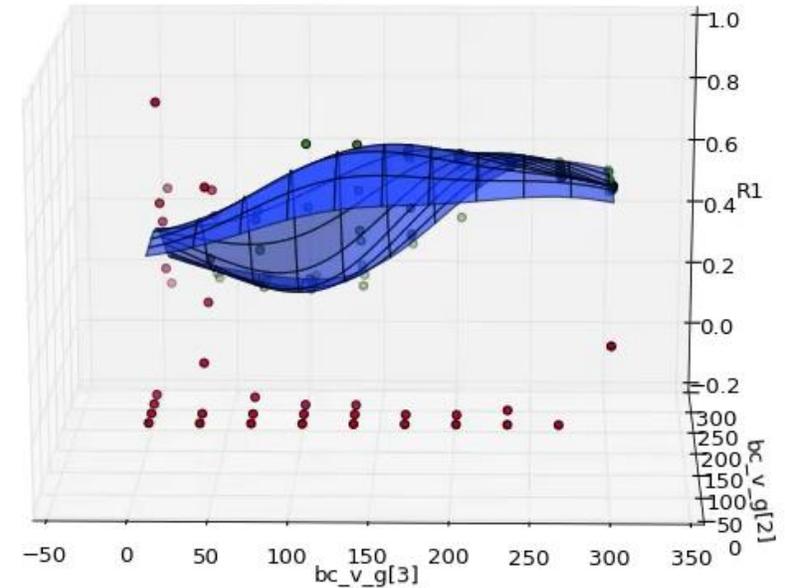
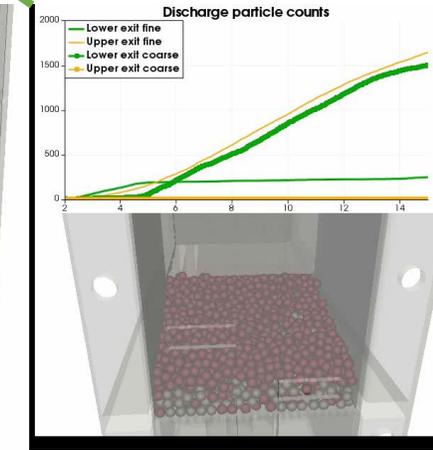
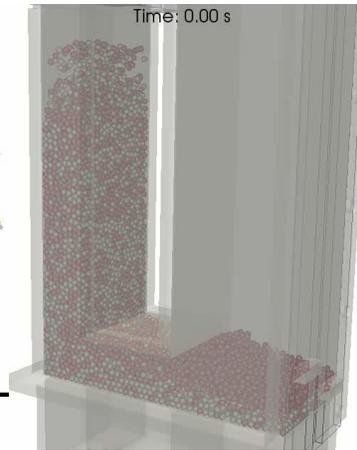
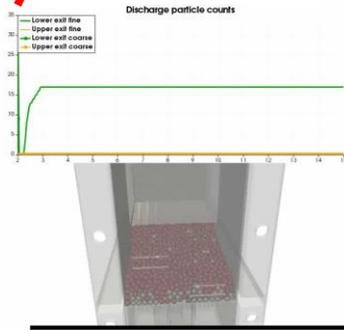
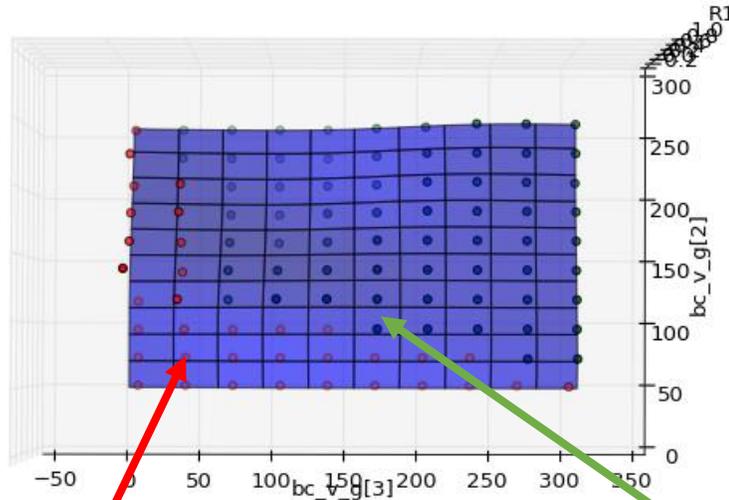
bc_v_g[2]

bc_v_g[3]



Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization



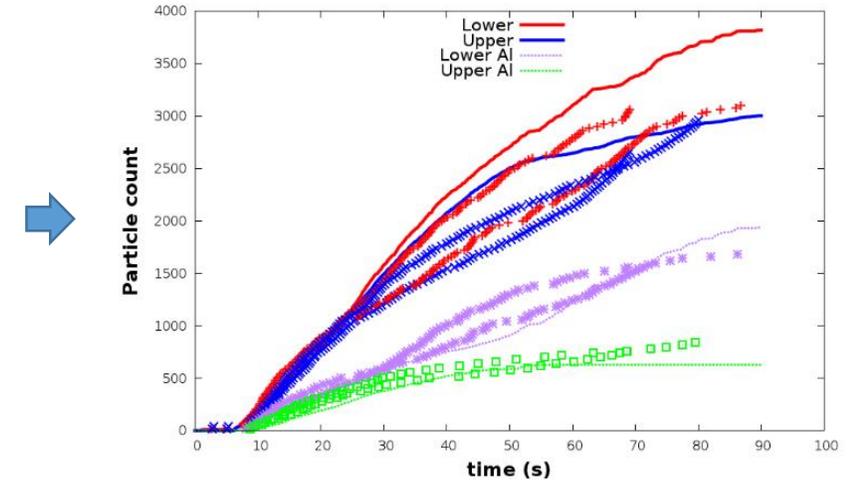
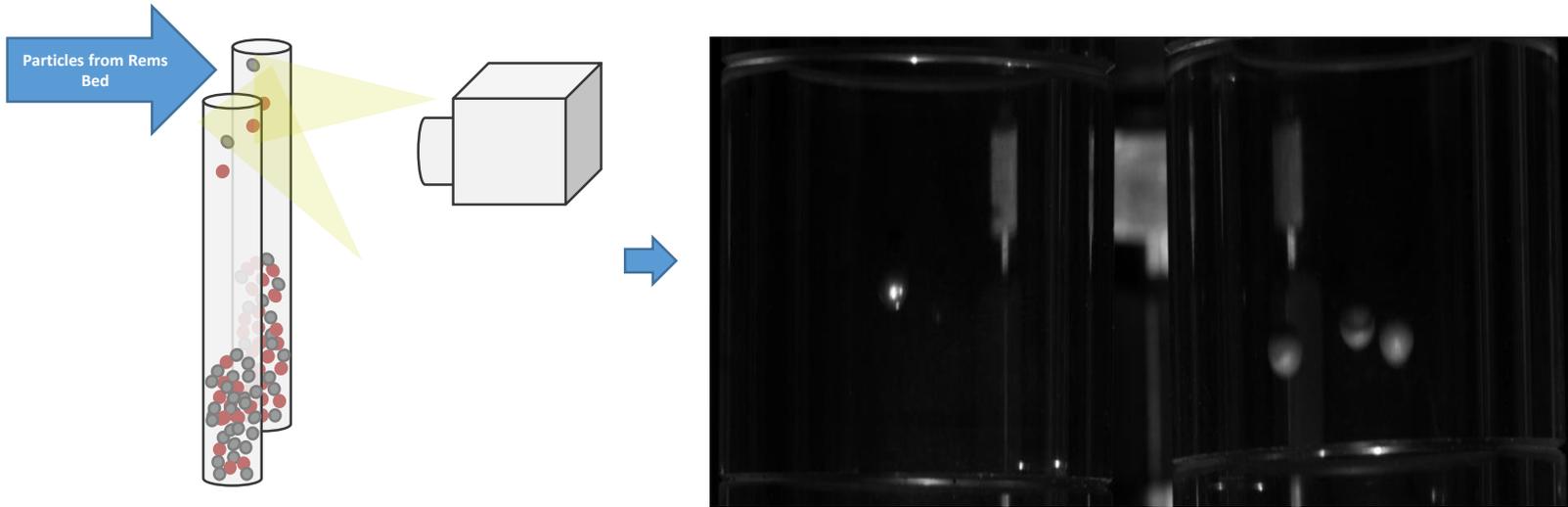
Optimum

$$bc_v_g[3] = 168.7$$

$$bc_v_g[2] = 95.4$$

Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization



- ✓ Particles are illuminated by high power light source and the back scattering is recorded using high speed camera at 250 frames/s
- ✓ The Aluminum particles scatters more light than Nylon beads and the optical setup is such that the reflection saturates the sensor
- ✓ The particles are tracked as they enter and leave the field of view, which covers the entire tube, and the number of trajectories provide the particle outflow rate
- ✓ The particle outflow rate is compared to CFD simulations

Advanced Applications

Novel CO2 Adsorber



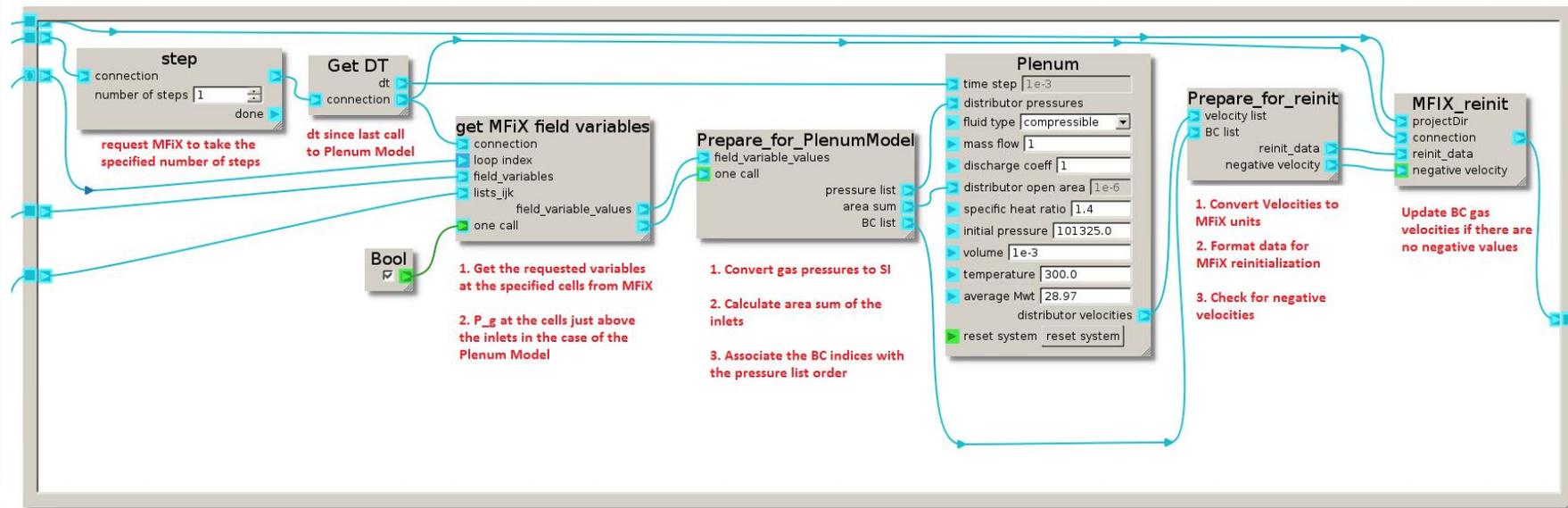
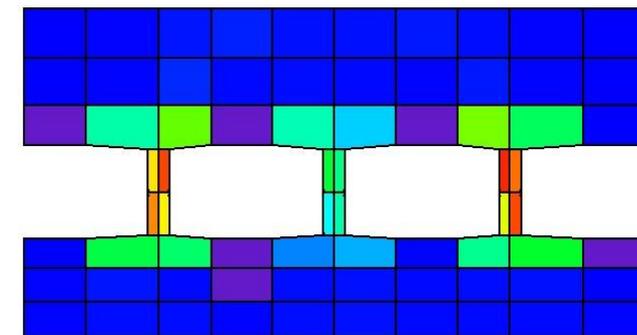
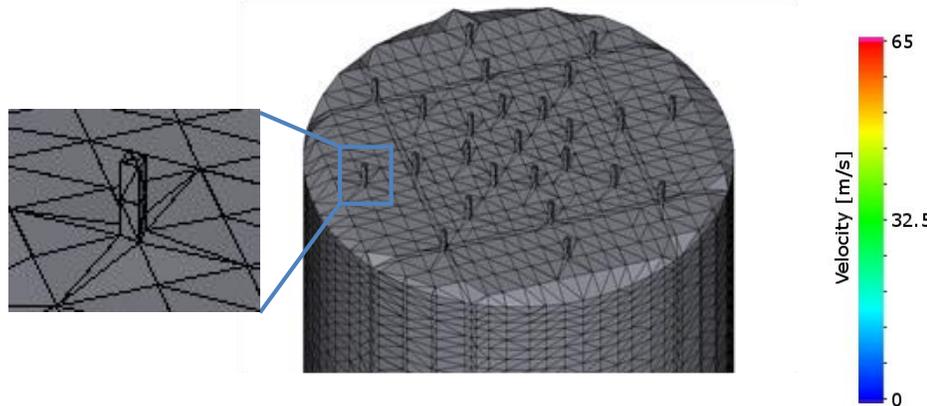
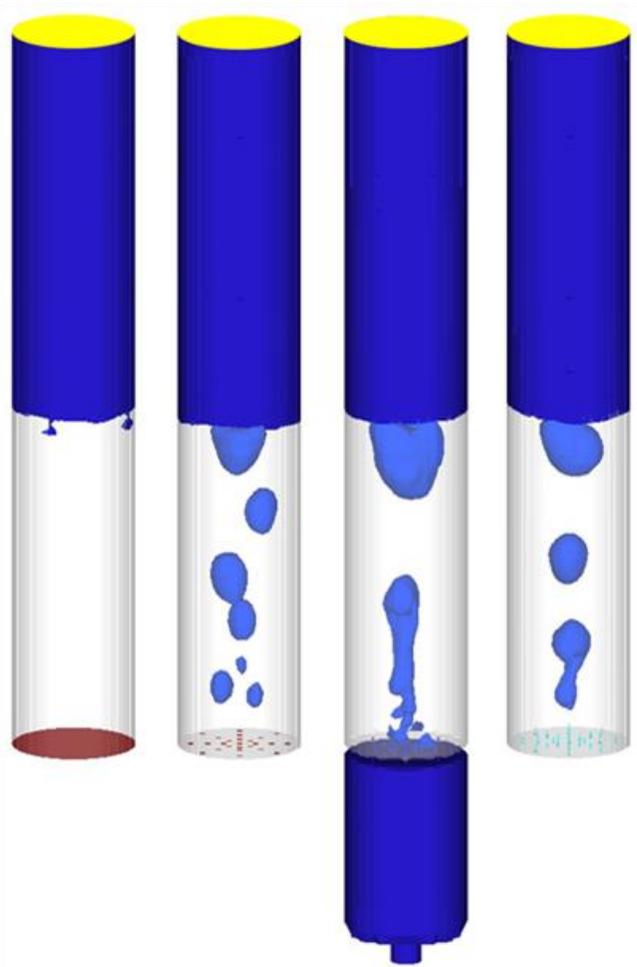
- Applied the OT to a Novel Heat/Pressure integrated CO2 Adsorber
- Uses NETL 32D Sorbent
- Used the OT to identify conditions for
 - >90% capture
 - >70% concentration by mass
 - <10% energy consumption
- Currently filing a patent for the design



thank you!

Further Application: Interactive MFiX

The REMS Toolset



Further Application: Process Modeling

The REMS Toolset



Stream

temperature 973.0
pressure 101325.0
flow rate [0.00035166666, 0.000259055555556]

Phase0 Phase1

database C:/python_projects/biomass_stream.cti

ideal gases
gas

Load from CTI

C6H10O5

	0	1	2
0	C6H10O5	0.30666963379	calculated
1	CO2	0.113445235464	calculated
2	CO	0.080634356546	calculated
3	CH2O	0.0542568972368	calculated
4	H2O	0.152797624171	calculated
5	CH3COOH	0.0411751947607	calculated

CTI Reaction

database /kbuchheit/Desktop/Christos Altantzis/ranzi1212_Orig.cti

ElementaryReaction : AC3H4 + AC3H4 => C2H4 + C4H4

	Reaction
0	ElementaryReaction : AC3H4 + AC3H4 => C2H4 + C4H4
1	ElementaryReaction : AC3H4 + CH3 <=> CH4 + C3H3
2	ElementaryReaction : AC3H4 + H <=> C3H3 + H2
3	ElementaryReaction : AC3H4 + OH <=> C3H3 + H2O
4	ElementaryReaction : AC3H4 <=> PC3H4
5	ElementaryReaction : C + O2 <=> CO + O

SS CSTR

Isothermal

temp 973.00
volume 0.001153

initial guess
reactions
input streams
parallel workers

assimulo
Cvode

abs tol 1e-18
rel tol 1e-10

Initialize with result
output stream
q 2323.79550685

SS PFR

Isothermal

temp 973.00
volume 0.006493

reactions
input streams
parallel workers

scipy
Isoda

abs tol 1e-18
rel tol 1e-10
length 1.0

output stream
q

Flow data
Temp data
volume data

Stream to CTI

stream
file TR973.cti

Print Stream

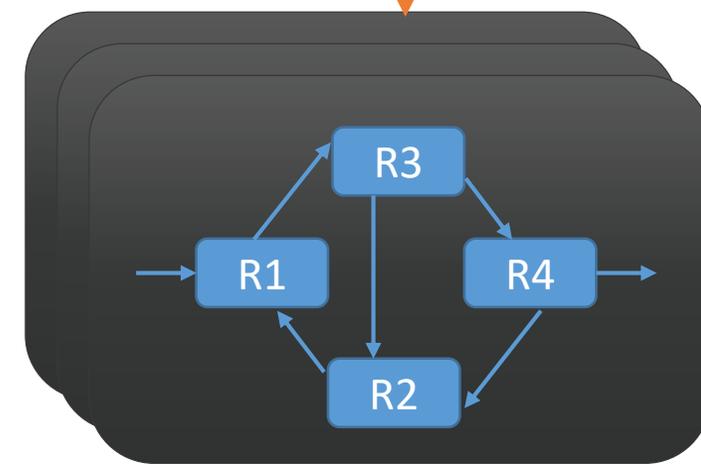
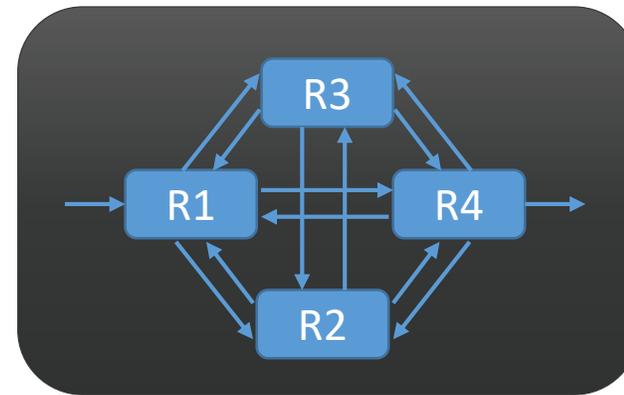
stream

Stream DataFrames

stream
outlet DataFrames

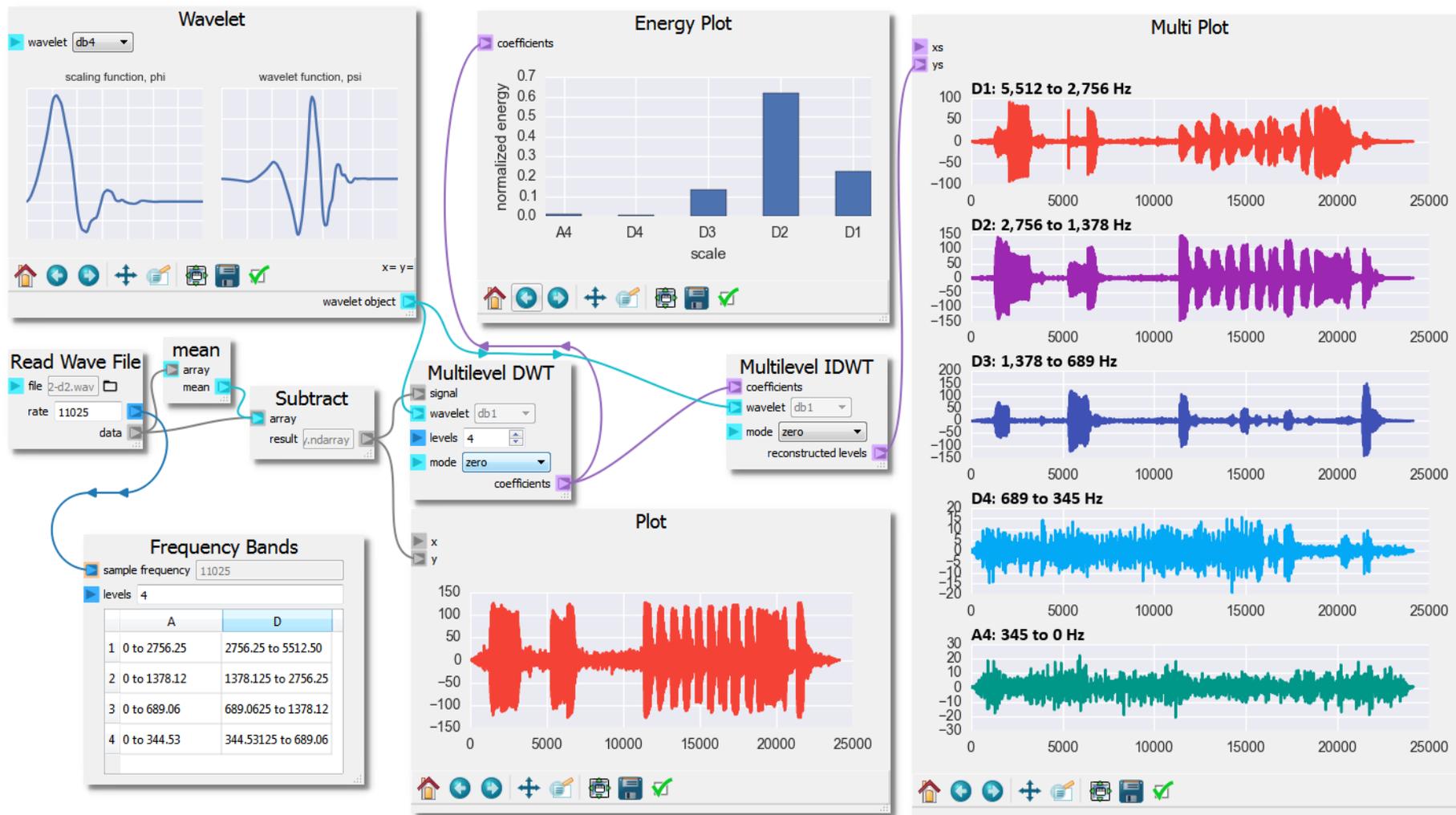
Save DataFrames

DataFrames
file othreact.xls



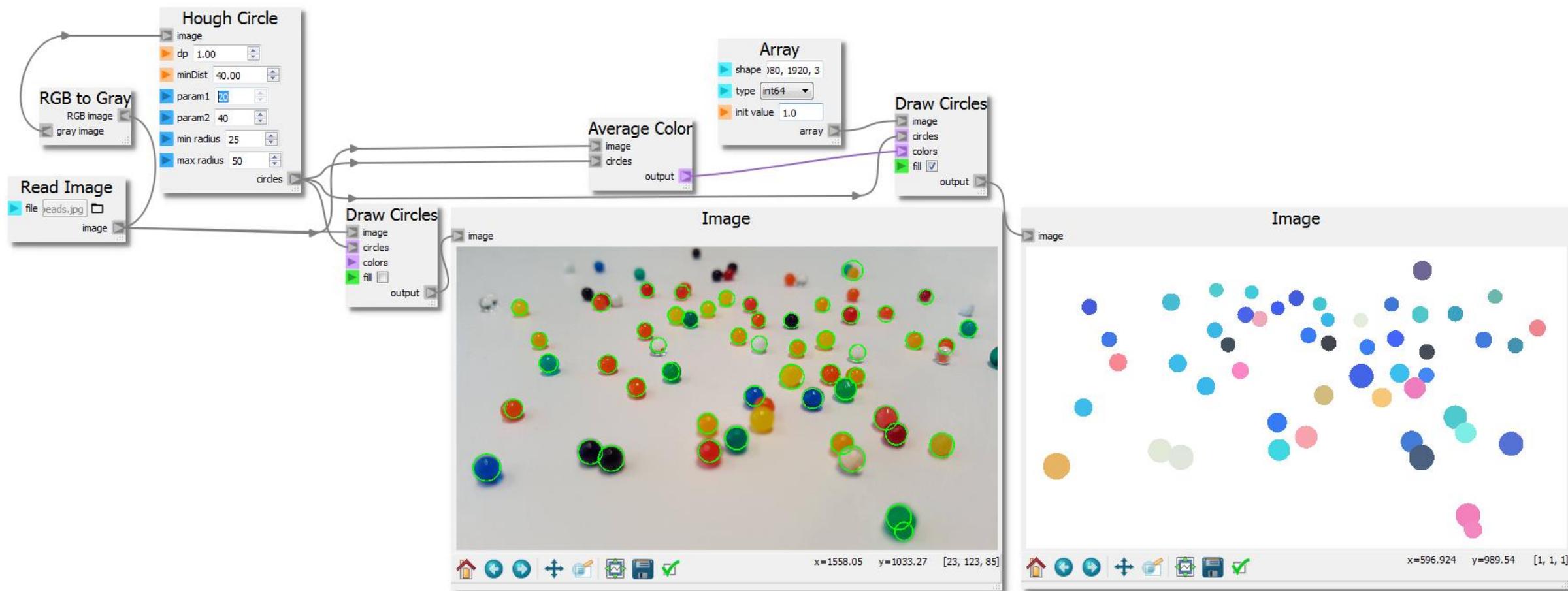
Further Applications: Signal Processing

The REMS Toolset



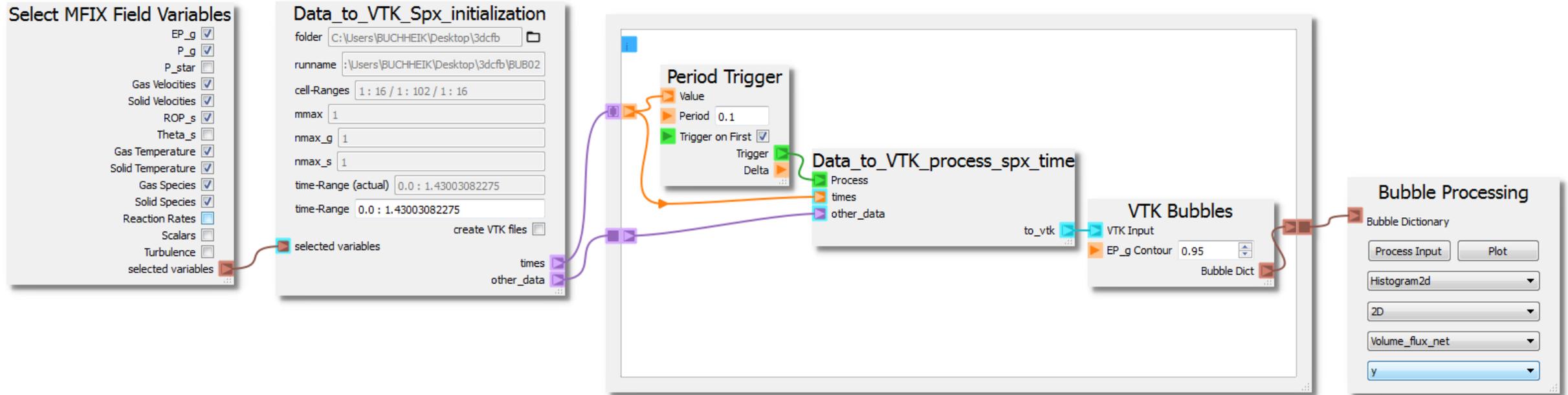
Further Applications: Image Analysis

The REMS Toolset



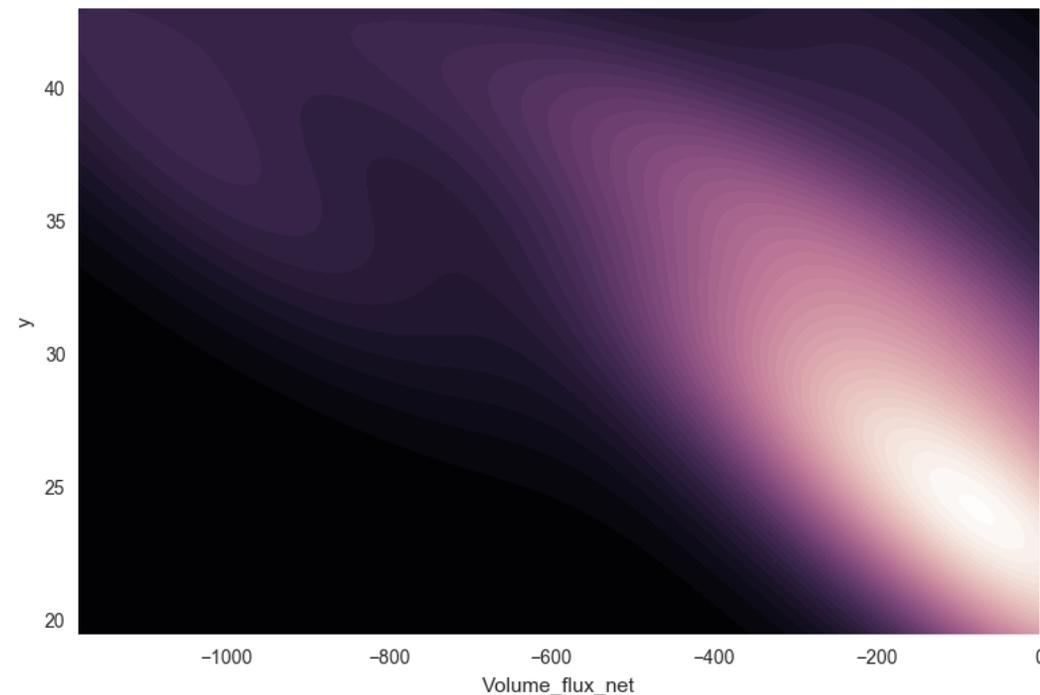
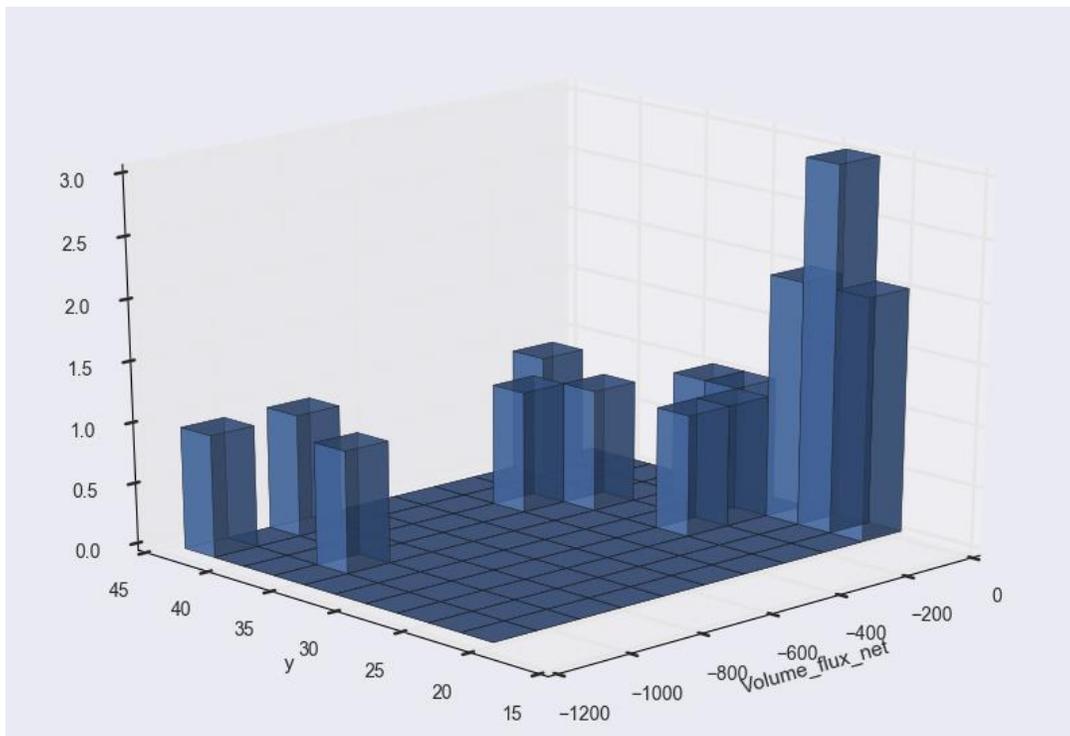
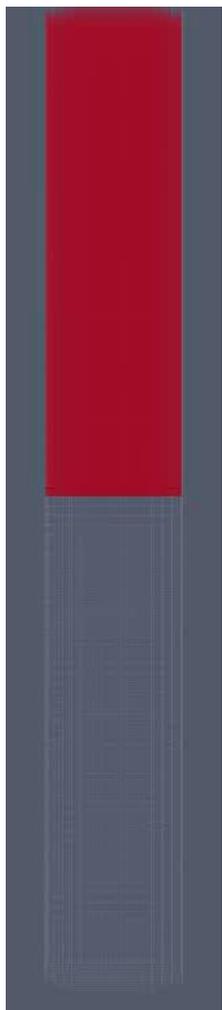
Further Applications: Bubble Analysis

The REMS Toolset



Further Applications: Bubble Analysis

The REMS Toolset



Complete MFS Team



MFS Team

S. Benyahia	A. Konan	M. Shahnam
G. Breault	T. Li	R. Singh
K. Buchheit	L. Lu	M. Syamlal
J. Carney	M. Meredith	J. Tucker
J. Dietiker	J. Musser	D. Van Essendelft
J. Finn	R. Panday	A. Vaidheeswaran
R. Garg	W. Rogers	V. Verma
A. Gel	P. Saha	J. Weber
B. Gopalan		Y. Xu
C. Guenther		K. Yoo
D. Huckaby		
T. Jordan		

Collaborators (PI)

G. Ahmadi (Clarkson)
I. Celik (WVU)
H. Emady (ASU)
C. Hrenya (UCB)
J. Hu (SNL)
V. Kumar (UTEP)
S. Mohaghegh (WVU)
J. De Wilde (UCL)
C. Roy (VT)
W. Spatz (SNL)
D. Tafti (VT)
C. Tong (LLNL)

