Predictive Analytics and Uncertainty Quantification of a Microscale Porous Reactor Simulation

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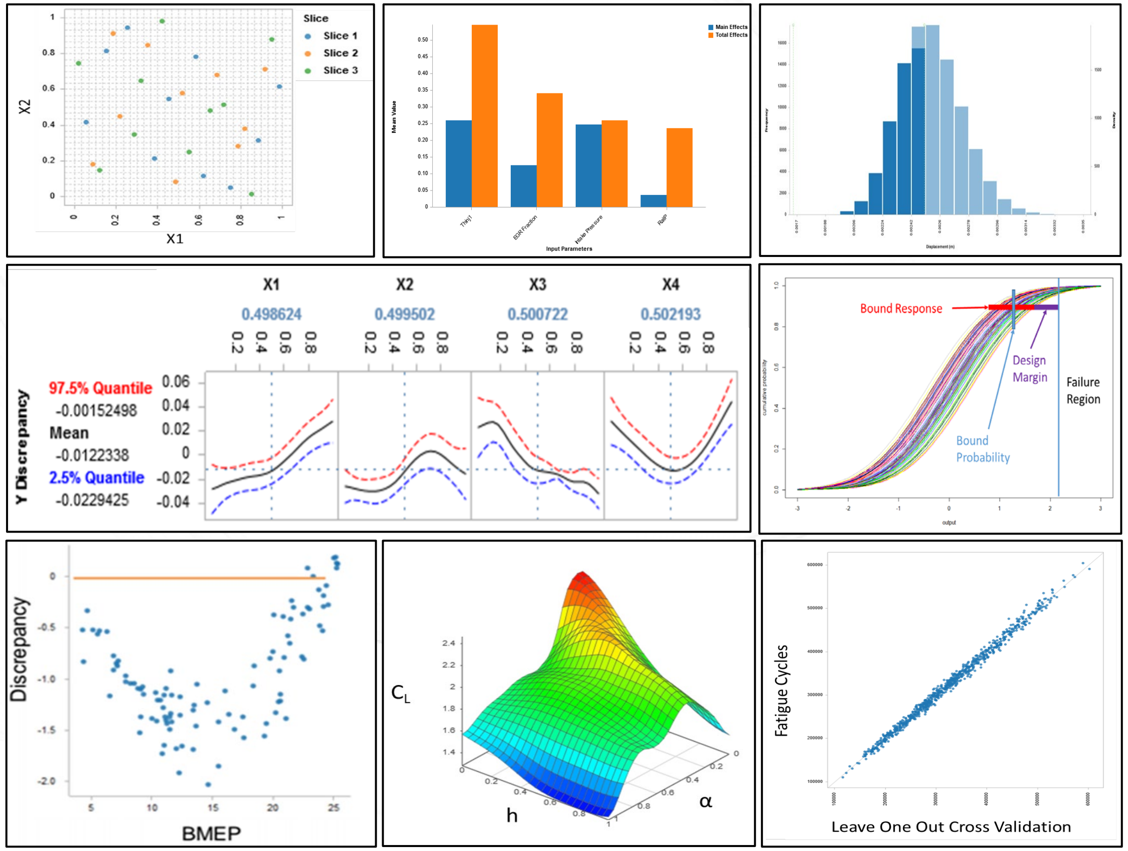
- **Who we are:** A Predictive Analytics and Uncertainty Quantification company based in Madison, WI.
- **Our Mission:** To deliver innovative software solutions that solve difficult problems in engineering and industrial applications.
- **Our Customers:** Engineering, testing, and analysis groups within industry and government.



What is Predictive Analytics?

Predictive Analytics encompasses a set of statistical tools used to analyze and extract information from data for the purpose of developing predictive models[1].

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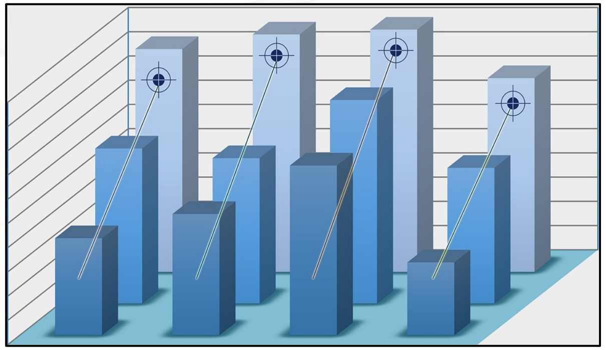

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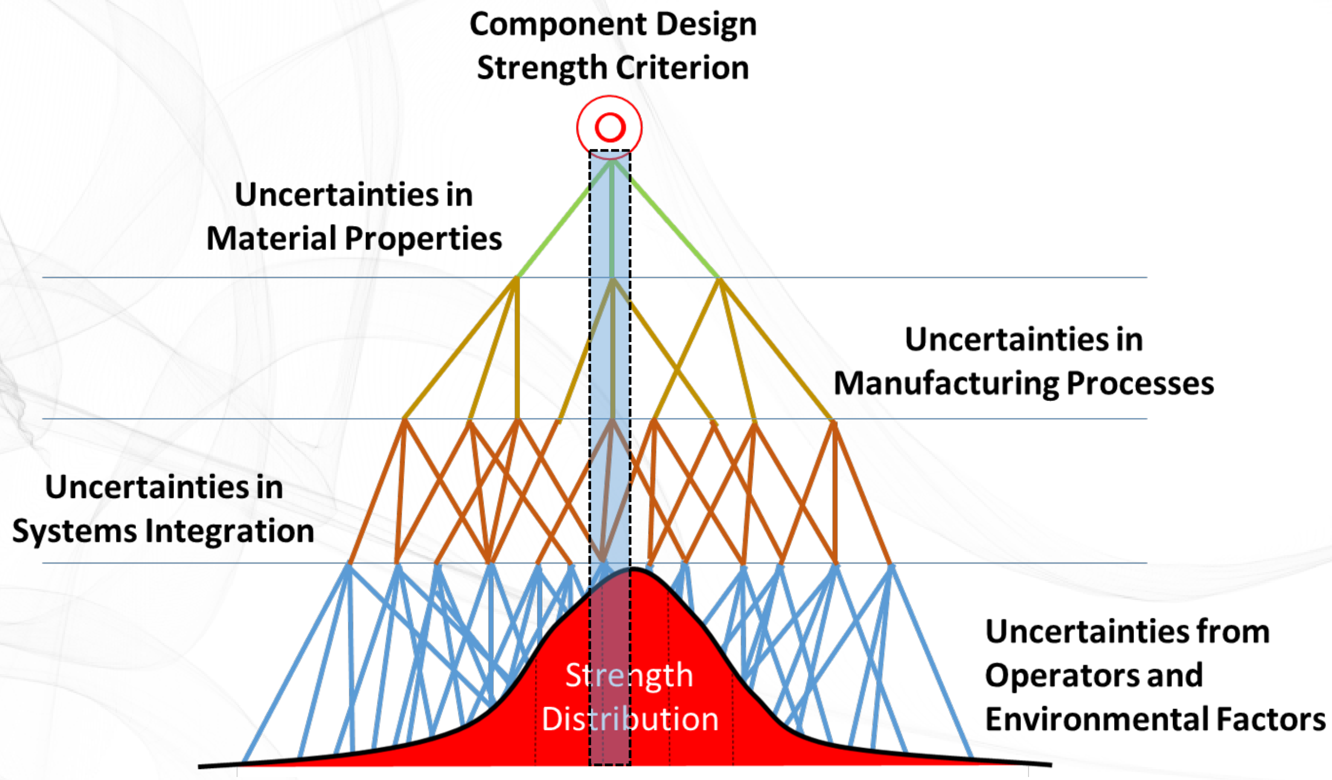
[1] https://en.wikipedia.org/wiki/Predictive_analytics

What is Uncertainty Quantification (UQ)?

Formulation of a statistical model to characterize imperfect and/or unknown information in engineering simulation and physical testing for predictions and decision making.

– NAFEMS Stochastics Working Group and ASME V&V 10 Definition.

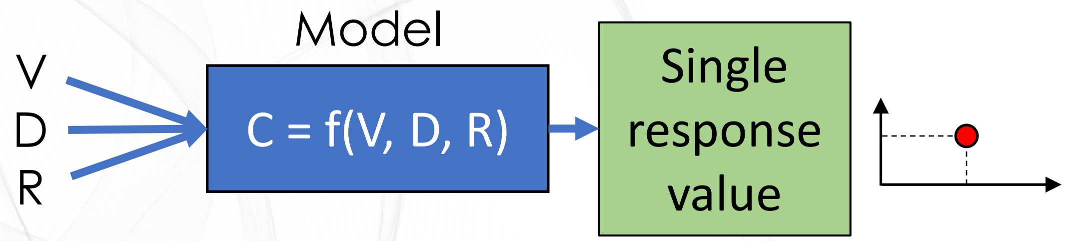


Objective: How likely are certain outcomes if some aspects of the complex system are not exactly known?

Deterministic Vs. Probabilistic Analysis

A **Deterministic** analysis assumes certainty in all aspects. It is meant to yield a single solution describing the outcome of some "experiment" given appropriate inputs.

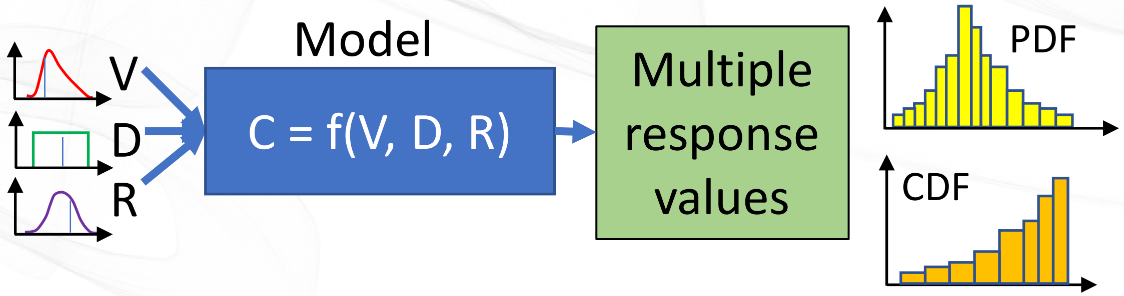
Single value parameter inputs



Examples:
timetables, pricing structures and maps.

A **Probabilistic** analysis is meant to give a distribution of possible outcomes. It describes all outcomes and gives some measure of how likely each is to occur.

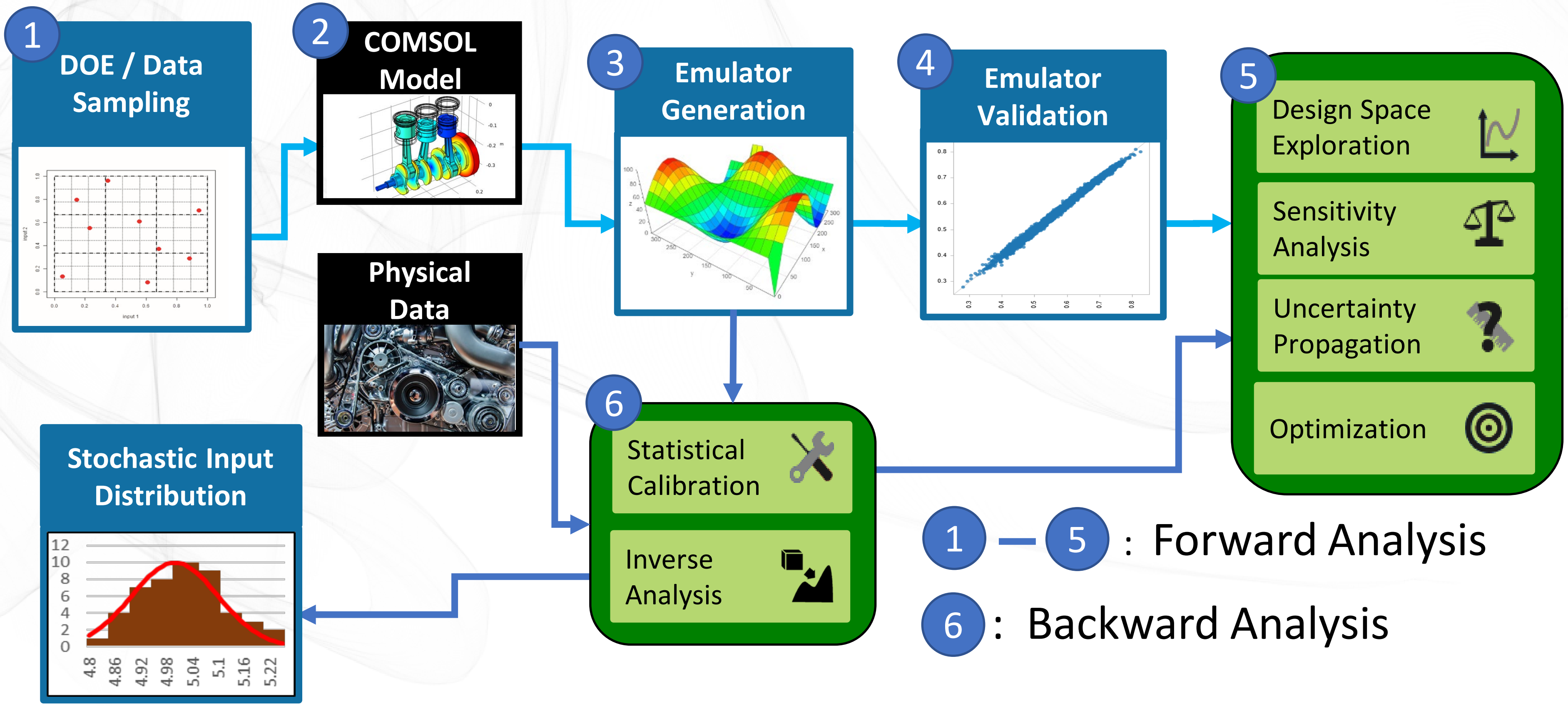
Multi-value parameter inputs



Examples:
fatigue of materials, residual stress field from welding and clinical drug trials.

Predictive Analytics & UQ Workflow Using SmartUQ Coupled to COMSOL

1. **Design of Experiments/Data Sampling** – Methods to minimize the number of simulations or tests needed; parse existing large data sets into manageable batches.
2. **Predictive Model Generation** – Build a predictive statistical model (a.k.a emulator or surrogate model) of the physics-based system for efficient design exploration and analysis.
3. **Analytics** – Tools to extract valuable information about the system that can be used to reduce technical risk.



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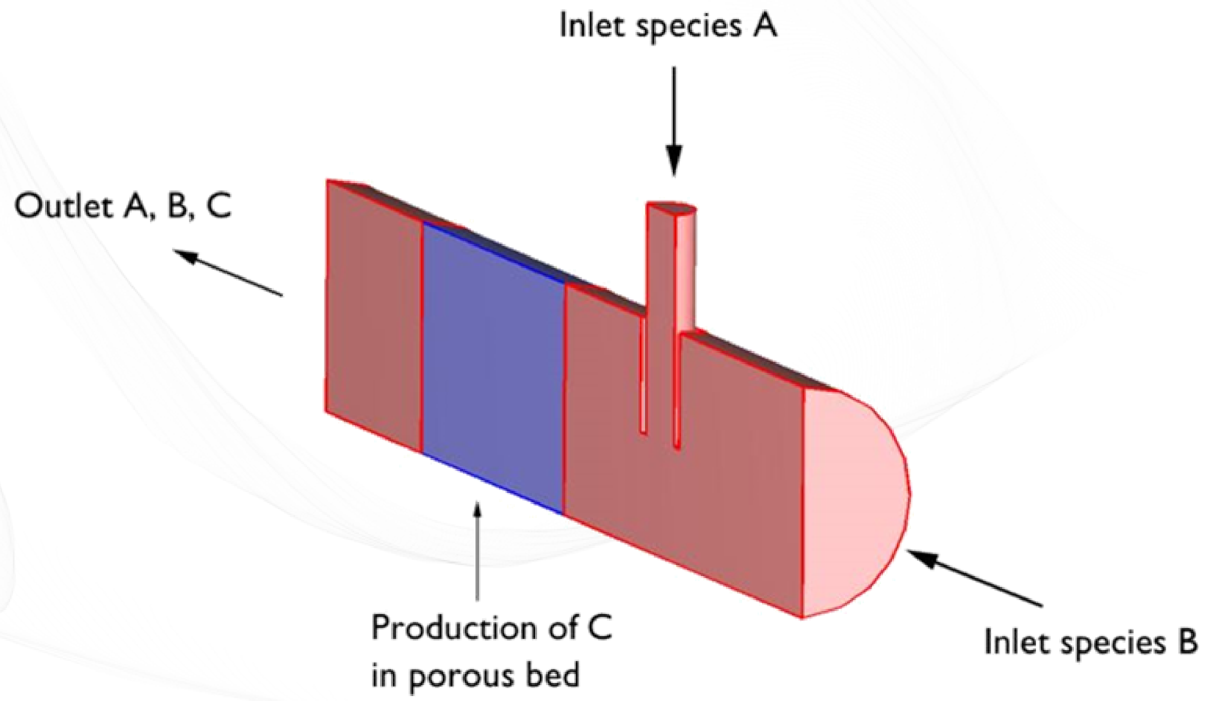
Microscale Porous Reactor Case Study Introduction

- A microscale porous reactor is used to catalyze a reaction that produces species C.
- The steady-state reacting flow is simulated using COMSOL Multiphysics
- 20 total input parameters



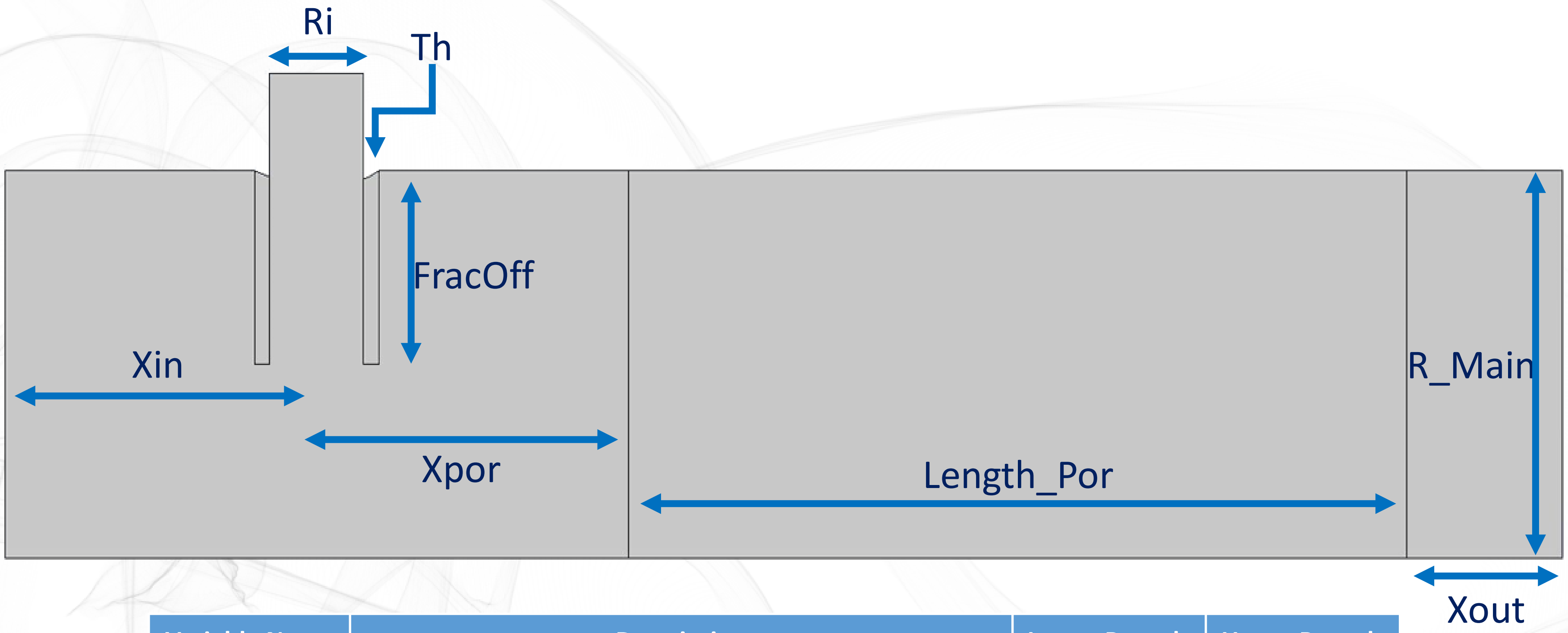
Output Parameters:

- Outlet velocity
- Exit concentrations of A, B, and C
- Pressure difference across the reactor

Goals:

- Determine the parameter values that produce species C at a concentration of 2.0 mol/m^3 at the outlet
- Determine the probability that the reactor will produce species C at a concentration between 1.8 mol/m^3 and 2.2 mol/m^3

8 Geometric Parameters



Variable Name	Description	Lower Bounds	Upper Bounds
R_Main	Radius of reactor	0.8 [mm]	1.2 [mm]
Ri	Inner radius of injection needle	0.175 [mm]	0.275 [mm]
Th	Annular thickness of injection needle	.05[mm]	0.1[mm]
Xin	Distance from the inlet to the injection site	0.75[mm]	2.0 [mm]
Xpor	Distance from the injection site to the reaction bed	.75 [mm]	2.0 [mm]
Xout	Distance from the end of the reaction bed to the outlet	.25 [mm]	2.0 [mm]
Length_por	Length of the porous reaction bed	1.0 [mm]	3.0 [mm]
FracOff	Radial distance of the injection site	0.4 [-]	0.6 [-]

Physics-based Parameters

Variable Name	Description	Lower Bounds	Upper Bounds
U0_A	Inlet velocity of species A	7.5 [cm/s]	12.5 [cm/s]
U0_B	Inlet velocity of species B	0.5 [cm/s]	1 [cm/s]
CA_0	Inlet concentration of species A	7.5 [mol/m^3]	15.0 [mol/m3]
CB_0	Inlet concentration of species B	2.5 [mol/m3]	5 [mol/m3]
T_iso	Temperature	290 [K]	310 [K]
A_f	Frequency factor	9.8e5 [m^3/(mol·s)]	1.2e6 [m^3/(mol·s)]
E	Activation energy	28,000 [J]	32,000 [J]
DA	Dissipation rate of species A in catalyst bed	9.5e-7 [m^2/s]	1.5e6 [m^2/s]
DB	Dissipation rate of species B in catalyst bed	9.5e-7 [m^2/s]	1.5e6 [m^2/s]
DC	Dissipation rate of species C in catalyst bed	9.5e-7 [m^2/s]	1.5e6 [m^2/s]
EpP	Porosity of catalyst bed	0.25 [-]	0.35 [-]
Kappa	Permeability of catalyst bed	9.5e10 [m^2]	1.5e10 [m^2]

Optimization

Goal

- For a reactor with R_Main of 1 mm and T_iso of 300 K
  - Achieve outlet concentration for species C of 2.0 mol/m^3
  - Minimize outlet concentrations for species A and B.

Constraints

- X_in > 1 mm
- X_out > 1 mm
- Underlying reaction physics parameters are fixed

Fixed Parameters	
Variable	**Value**
R_Main	1 [mm]
T_iso	300 [K]
A_f	1,090,000 [m^3/(mol*s)]
E	30,000 [J/mol]
DA	1.225e-6 [mol^2/s]
DB	1.225e-6 [mol^2/s]
DC	1.225e-6 [mol^2/s]
EpP	0.3 [-]
Kappa	1.22e-9[m^2]

Optimization Results

Optimized Parameters	
Variable	Value
Length_por	2.4538 [mm]
Xin	1.8937 [mm]
Xpor	1.9263 [mm]
Xout	1.6607 [mm]
Ri	0.1930 [mm]
Th	0.0746 [mm]
FracOff	0.4323 [-]
U0_A	9.2514[cm/s]
U0_B	0.6994 [cm/s]
C0_A	9.7987 [mol/m^3]
C0_B	3.3418 [mol/m^3]

Optimized Outputs	
Output	Value
V_{out}	0.1070 [cm/s]
C_A	1.1851 [mol/m^3]
C_B	0.2476 [mol/m^3]
C_C	**2.0002 [mol/m^3]**
Δ_P	0.4316 [Pa]

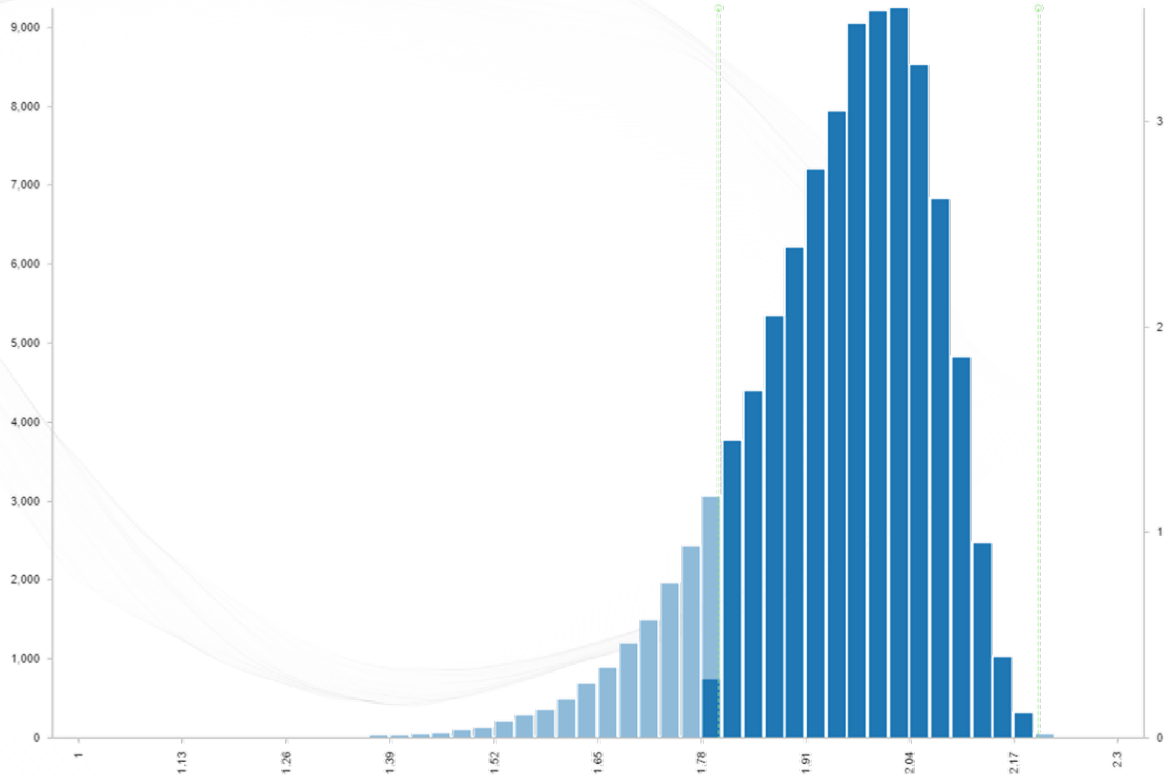
Uncertainty Propagation

Goal

- Determine the probability under uncertainty that the optimized reactor will produce species C at a concentration between 1.8 and 2.2 mol/m^3
- Uncertainty in optimized parameters normally distributed around optimum values
- Uncertainty in fixed parameters normally distributed around fixed values.

Results

- 100,000 points drawn from input uncertainty distributions and propagated using the emulator
- 87% chance concentration of C is between 1.8 and 2.2 mol/m^3



Output uncertainty distribution for concentration of C has mean of 1.95 mol/m^3 and standard deviation of 0.125 mol/m^3

For More Information on SmartUQ or Predictive Analytics. . .

- **COMSOL Conference Sponsor Presentation**
  - Coupling SmartUQ's Predictive Analytics and Uncertainty Quantification Solutions with COMSOL
- **Download SmartUQ white papers from our website:** http://www.smartuq.com/resources/whitepaper/
  - *Statistical Calibration: Grounding Simulations in Reality*
  - *Introduction to SmartUQ Analytics and Digital Twins*
- **On Demand Webinars:** http:// smartuq.com/resources/webinars
  - *Introduction to Uncertainty Quantification for Engineers*
  - *Introduction to Predictive Analytics for Engineers*

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