Optimization Under Uncertainty

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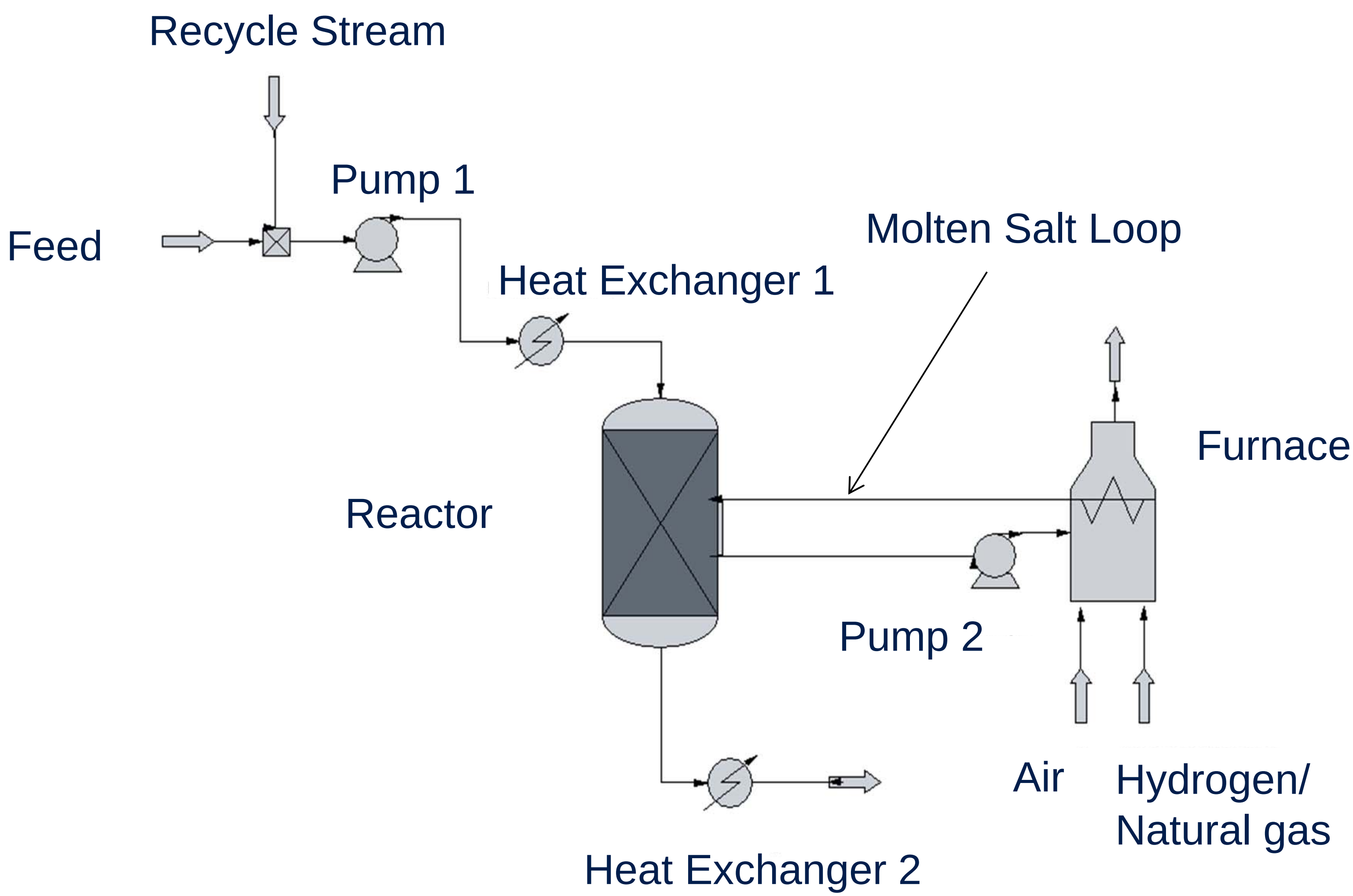
Overview

- Model
  - Description of Acetone Plant
- Optimization
  - Genetic Algorithm
  - Global Optimization
  - Using Uncertainty Descriptions in Optimization
- Conclusions

Acetone Reactor System

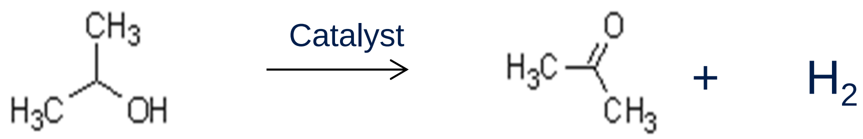


Model Size

- Steady-state design problem
- Parameters: 70
- Intermediates: 96
- Variables: 43 (+8 Design Parameters)
- Equations: 43
- Mixed Integer Nonlinear Programming (MINLP)
- GA developed in MATLAB
- APM as the NLP solver

Acetone Reaction

Dehydrogenation of isopropyl alcohol to form acetone and hydrogen



Parameter	Value
Cost of isopropyl alcohol	1.27 $/kg
Cost of acetone	1.80 $/kg
Cost of electricity	6.77 cents/kwh
Cost of natural gas	5.08 $/1000 ft^3
Cost of catalyst	351,500 $/$m^3$
Interest (i)	9 %
Number of years in operation (n)	20 yrs

Model Design

Objective function

$$NPV = -(p1_{Cbm} + hx1_{Cbm} + r_{Cbm} + f_{Cbm} + hx2_{Cbm} + p2_{Cbm}) + (cst_{acet} - cst_{IPA} - cst_{elec} - cst_{NG})\left(\frac{1-(1+i)^{-n}}{i}\right) - cst_{cat} * n$$

Design Variables	Range	Design Variables	Range
Initial flow rate of isopropyl alcohol	36-144 kmol/hr	Diameter of tubes in reactor	0.03-0.07 m
Conversion of isopropyl alcohol	0.85-0.92	Molten salt flow rate	9.5-40 kg/s
Temperature of vapor entering reactor	600-773.15 K	Diameter of tubes before reactor	0.25-3 in
Number of tubes in reactor	1-700	Diameter of tubes in the molten salt loop	0.25-2 in

Genetic Algorithm

- Based on evolution
- Diversity
- Inheritance
- Fitness

Similarities to Evolution

- Parents
- Chromosomes

p1_nIPA	XIPA	r_Thi	r_n	r_d	p2_mdot	p1_d	p2_d	NPV
0.0344	0.9134	621.9891	640	6	12.4750	0.75	1.75	7.9190

- Survival of the fittest

Diversity

- Initial population randomly dispersed throughout the design space
- Random mutation of genes
  - Uniform
  - Dynamic
- Tournament size

Parent Selection

- Tournament
- Randomly select x number of candidates
- One with best fitness selected as parent

Inheritance

- Crossover
  - Parents

p1_nIPA	XIPA	r_Thi	r_n	r_d	p2_mdot	p1_d	p2_d
0.0344	0.9134	621.9891	640	6	12.4750	0.75	1.75
0.0387	0.9175	627.2923	680	7	24.3039	1.75	0.5

  - Single-point

p1_nIPA	XIPA	r_Thi	r_n	r_d	p2_mdot	p1_d	p2_d
0.0344	0.9134	621.9891	640	7	24.3039	1.75	0.5
0.0387	0.9175	627.2923	680	6	12.4750	0.75	1.75

  - Uniform

p1_nIPA	XIPA	r_Thi	r_n	r_d	p2_mdot	p1_d	p2_d
0.0344	0.9175	621.9891	680	7	12.4750	1.75	1.75
0.0387	0.9134	627.2923	640	6	24.3039	0.75	0.5

Fitness and Elitism

- Fitness
  - Objective function
  - Used to eliminate infeasible designs

$$NPV = -(p1_{Cbm} + hx1_{Cbm} + r_{Cbm} + f_{Cbm} + hx2_{Cbm} + p2_{Cbm}) + (cst_{acet} - cst_{IPA} - cst_{elec} - cst_{NG})\left(\frac{1-(1+i)^{-n}}{i}\right) - cst_{cat} * n$$

- Elitism
  - Rank children and parents according to fitness
  - Keep best fits

Genetic Algorithm Design

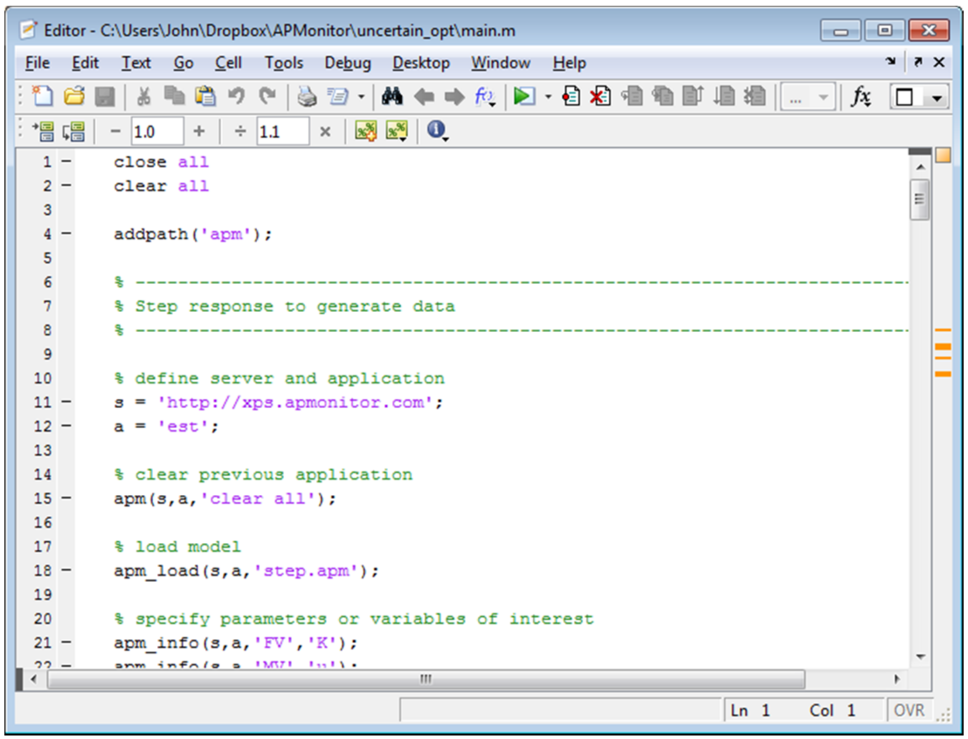
- Gene size: 8
- Generation size: 20
- Tournament size: 2
- Crossover probability: 30%
- Mutation rate: 10%
- Number of iterations: 50

Results

Variable	Average value from genetic algorithm	Standard deviation	99% Confidence	Sensitivity of NPV	Value from continuous solver
p1_nIPA	0.03989 kmol/s	7.3786e-5	6.55e-5	2.56e10	0.04 kmol/s
XIPA	0.91931	7.22e-4	6.41e-4	2.07e9	0.92
r_Thi	768.9792 K	3.724663	3.306242	6.825e4	773.15 K
r_n	435	191.5365	170.0197	0	700
r_d	5.3 cm	1.494434	1.326552	-3.97e8	3 cm
p2_mdot	39.00364 kg/s	0.876951	0.778436	-7667.8	14.907 kg/s
p1_d	1.2 in	0.57494	0.510352	4.8e7	2.992 in
p2_d	1.625 in	0.868028	0.770515	9.887e6	0.913 in
NPV	$10.288e8	0.020976	0.01862		$10.322e8

Example Application

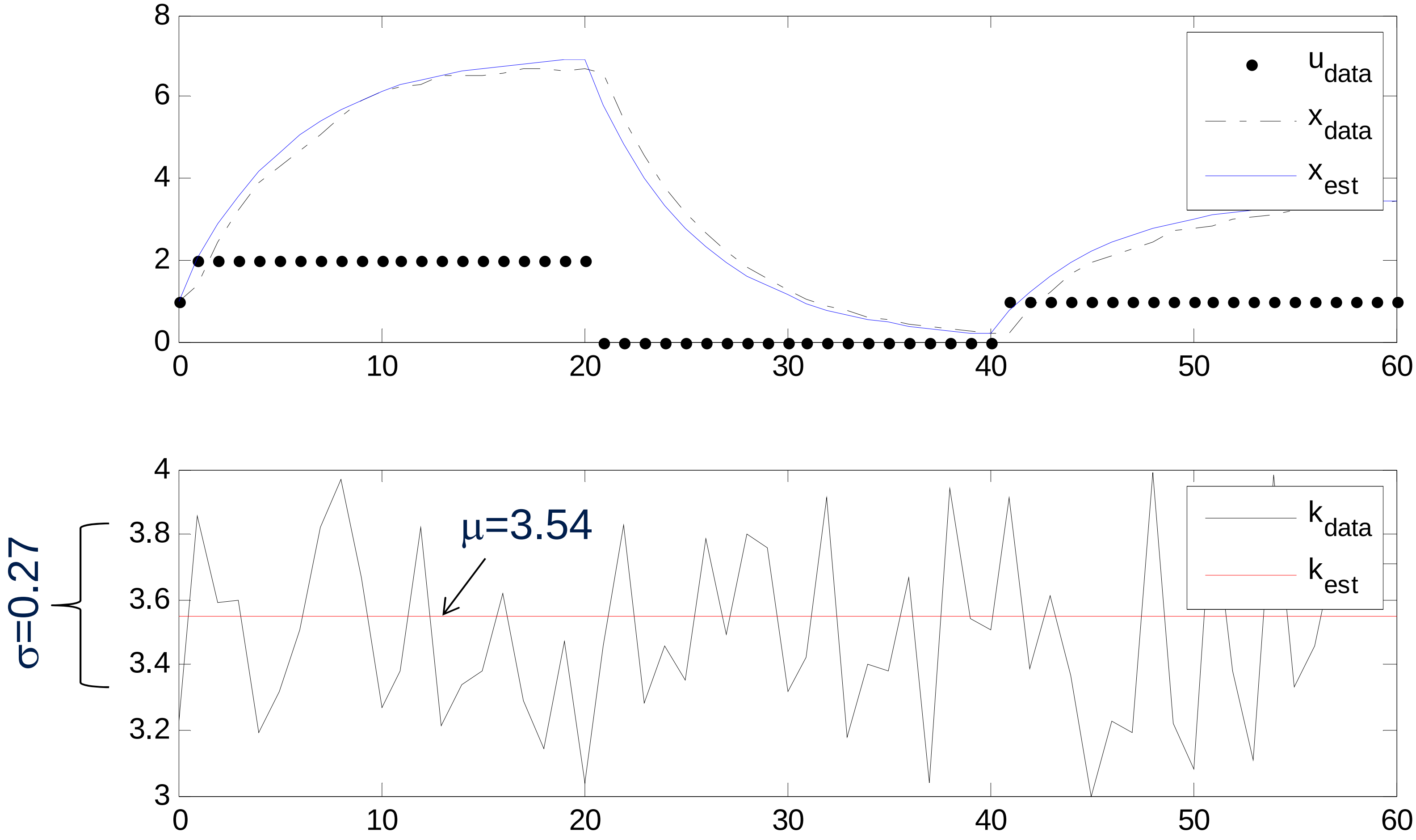
- Download Application:
  - http://apmonitor.com/wiki/uploads/Main/apm_uncertain_params.zip
- Open in MATLAB



Example Model

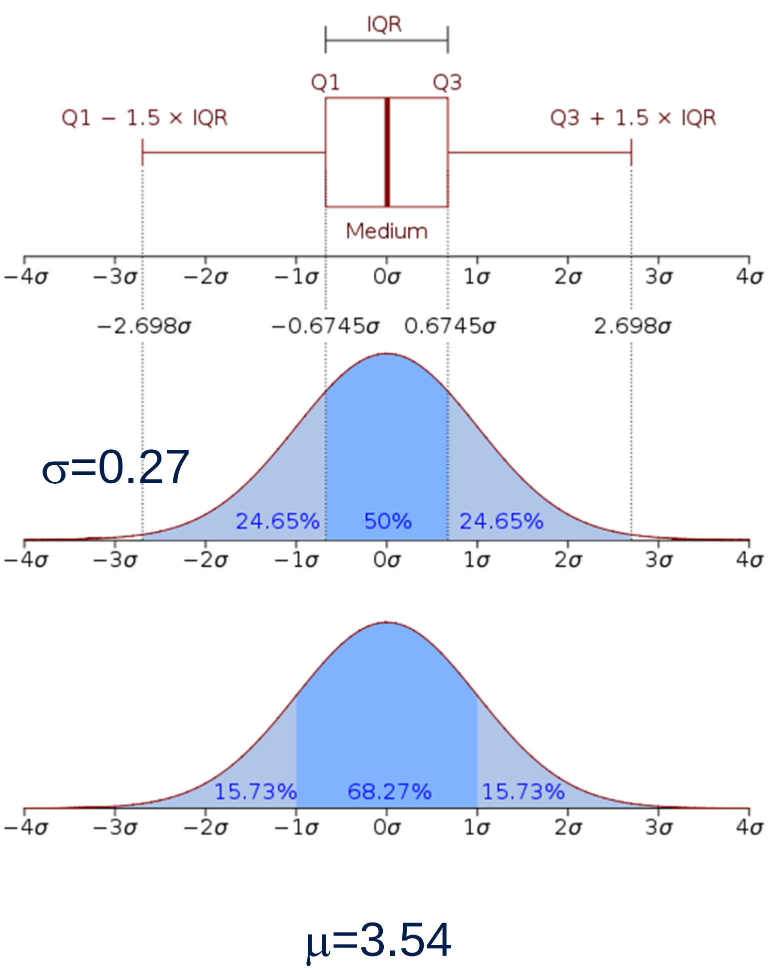
```
Model
  Parameters
    tau  = 5                    ! time constant (sec to 63.2% of a step change)
    K    = 2                    ! gain (change x / change u)
    u    = 1                    ! input or manipulated variable
  End Parameters

  Variables
    x = 1                       ! output or controlled variable
  End Variables

  Equations
    tau * $x = -x + K * u       ! first order differential equation
  End Equations
End Model
```

Determine Parameter Uncertainty



Using Parameter Uncertainty

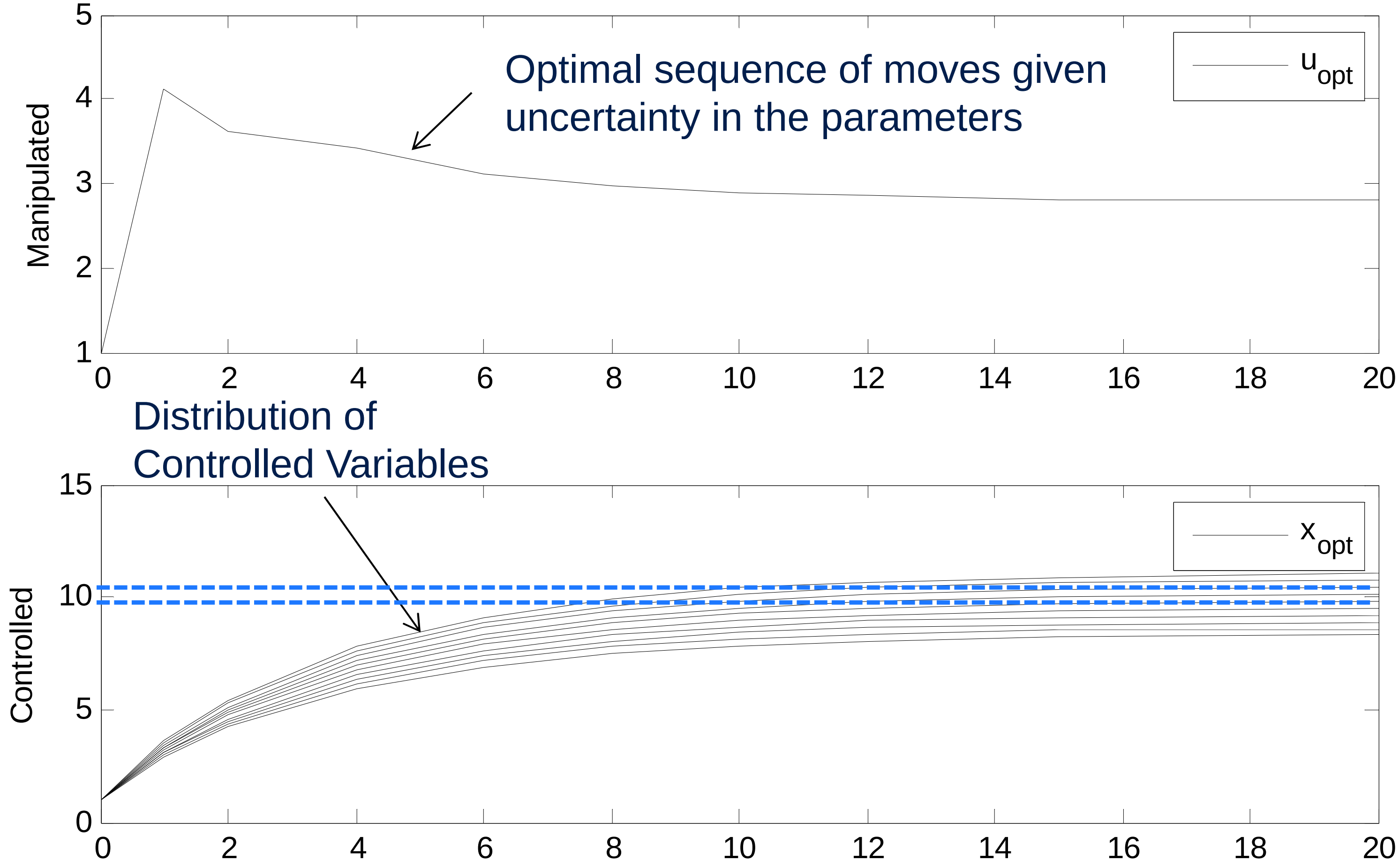
- Two Approaches
  - Generate cases that are representative of a given distribution
  - Create a sub-set of models that represent the distribution



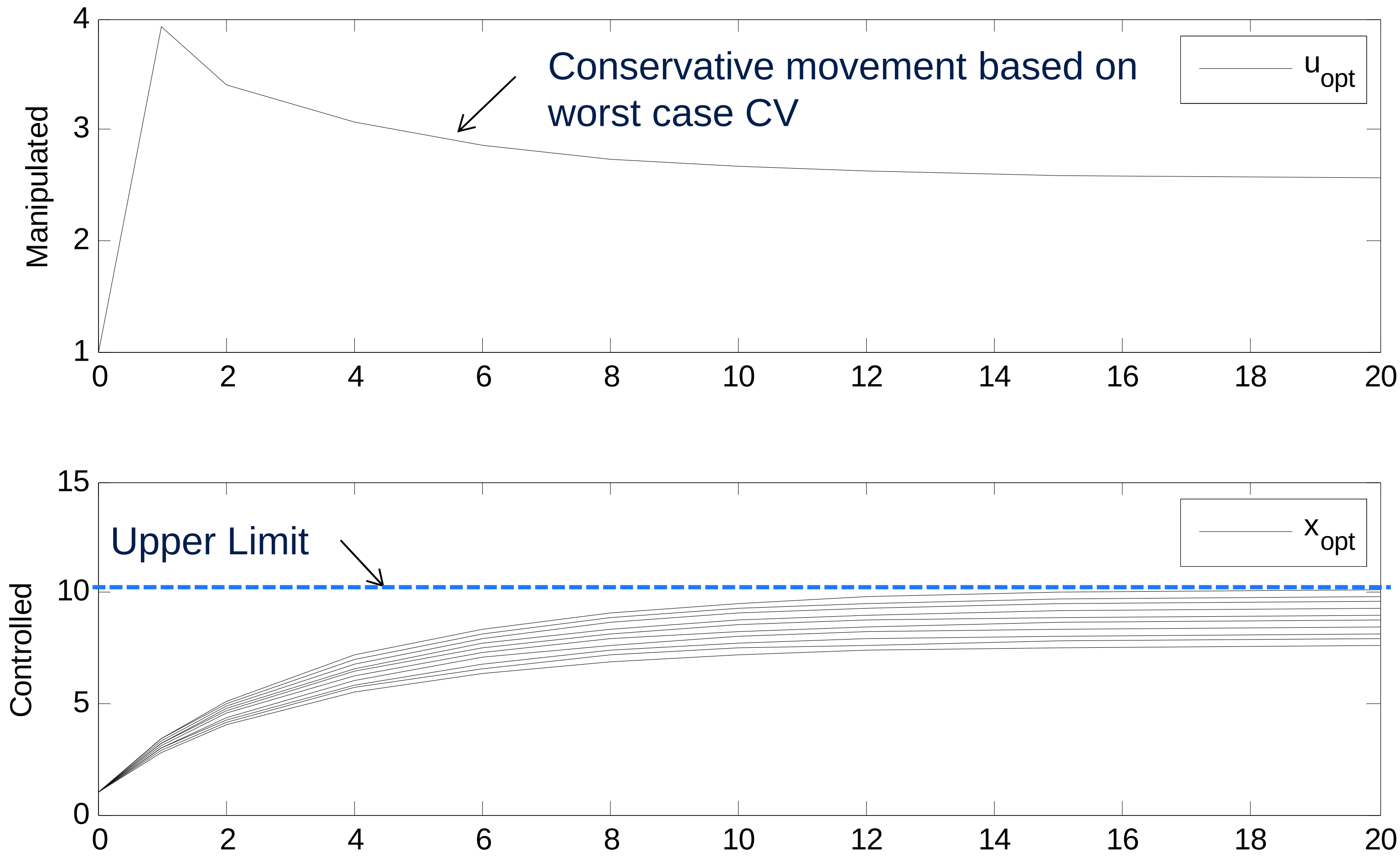
Example Model with Uncertainty

```
Model
  Constants
    n     = 10                  ! number of sampling points
  End Parameters

  Parameters
    tau    = 5                  ! time constant (sec to 63.2% of a step change)
    K[1:n] = 2                  ! gain (change x / change u)
    u      = 1                  ! input or manipulated variable
  End Parameters

  Variables
    x[1:n] = 1                  ! output or controlled variable
  End Variables

  Equations
    tau * $x[1:n] = -x[1:n] + K[1:n] * u       ! first order differential equation
  End Equations
End Model
```

Optimize to a Target Range



Optimize to a Limit



Conclusions

- Global Optimization Approach
  - Optimal Process Design for Maximum NPV
  - Parameter Uncertainty Calculated
  - Genetic Algorithm Finds a Global Optimum
- Optimization Under Uncertainty
  - Parameter Distribution Used in Control
  - Drive to Target or a Limit