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APPENDIX A

AQUASIM 2.0

Variables

A:  Description: Cross-sectional area
    Type:    Constant Variable
    Unit:    m²
    Value:   0.00046495435
    Standard Deviation: 1
    Minimum: 0
    Maximum: 1000
    Sensitivity Analysis: active
    Parameter Estimation: inactive

a:   Description: 
    Type:    Constant Variable
    Unit:    
    Value:   -66
    Standard Deviation: 1
    Minimum: -100
    Maximum: 10000
    Sensitivity Analysis: active
    Parameter Estimation: inactive

alpha: Description: 
    Type:    Formula Variable
    Unit:    
    Expression: 0.5

b:   Description: 
    Type:    Constant Variable
    Unit:    days
    Value: 3.030879
    Standard Deviation: 1
    Minimum: 0
    Maximum: 1000
    Sensitivity Analysis: active
    Parameter Estimation: inactive

C:   Description: Dissolved concentration
    Type:    Dyn. Volume State Var.
    Unit:    mg/m³
    Relative Accuracy: 1e-006
    Absolute Accuracy: 1e-006

C5:   Description: 
    Type:    Constant Variable
Unit: mg/L
Value: 4.02255
Standard Deviation: 1
Minimum: 0
Maximum: 55
Sensitivity Analysis: active
Parameter Estimation: inactive

<table>
<thead>
<tr>
<th>Description</th>
<th>Type</th>
<th>Unit</th>
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</thead>
<tbody>
<tr>
<td>calcnum</td>
<td>Program Variable</td>
<td></td>
</tr>
<tr>
<td>Cmeas</td>
<td>Real List Variable</td>
<td>mg/L</td>
</tr>
<tr>
<td>Co</td>
<td>Initial added added chromium</td>
<td></td>
</tr>
<tr>
<td>C_crit</td>
<td>Formula Variable</td>
<td>mg/m³</td>
</tr>
<tr>
<td>C_in</td>
<td>Formula Variable</td>
<td>mg/L</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Type</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Program Variable</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Real List Variable</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Formula Variable</td>
<td></td>
<td>50</td>
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<tr>
<td>Formula Variable</td>
<td></td>
<td>0.01</td>
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<tr>
<td>Formula Variable</td>
<td></td>
<td>50</td>
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<table>
<thead>
<tr>
<th>Time</th>
<th>Cmeas</th>
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<tbody>
<tr>
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<td>0</td>
</tr>
<tr>
<td>0.0938</td>
<td>36.6697</td>
</tr>
<tr>
<td>0.8438</td>
<td>34.4415</td>
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<tr>
<td>1.0208</td>
<td>35.0144</td>
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<td>1.1146</td>
<td>35.651</td>
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<tr>
<td>38.0063</td>
<td>5.2203</td>
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<td>39.9646</td>
<td>4.3927</td>
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<tr>
<td>42.1417</td>
<td>5.1567</td>
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<tr>
<td>43.1</td>
<td>3.2468</td>
</tr>
<tr>
<td>45.1</td>
<td>3.1195</td>
</tr>
</tbody>
</table>

Interpolation Method: linear interpolation
Real Data Pairs (65 pairs):
### C_in_meas

**Description:** Real List Variable

**Type:** Real List Variable
**Unit:** mg/L

**Argument:** t

**Standard Deviations:** global

**Rel. Stand. Deviat.:** 0

**Abs. Stand. Deviat.:** 1

**Minimum:** 0

**Maximum:** 1e+009

**Interpolation Method:** linear interpolation

**Sensitivity Analysis:** inactive

**Real Data Pairs (65 pairs):**

<table>
<thead>
<tr>
<th>t</th>
<th>C_in_meas</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>47.937929</td>
</tr>
<tr>
<td>0.09375</td>
<td>47.937929</td>
</tr>
<tr>
<td>0.84375</td>
<td>47.746941</td>
</tr>
<tr>
<td>1.0208333</td>
<td>48.383567</td>
</tr>
<tr>
<td>1.1145833</td>
<td>45.837064</td>
</tr>
<tr>
<td>38.00625</td>
<td>50.102457</td>
</tr>
<tr>
<td>39.964583</td>
<td>45.773401</td>
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<tr>
<td>42.141667</td>
<td>50.038794</td>
</tr>
<tr>
<td>43.1</td>
<td>48.95653</td>
</tr>
<tr>
<td>45.1</td>
<td>48.383567</td>
</tr>
</tbody>
</table>

### D

**Description:** Dispersion coefficient

**Type:** Constant Variable
**Unit:** m²/h

**Value:** 4.0990701

**Standard Deviation:** 4.0990701

**Minimum:** 0

**Maximum:** 10

**Sensitivity Analysis:** active

**Parameter Estimation:** inactive

### K

**Description:** half velocity

**Type:** Formula Variable
**Unit:** mg/m³

**Expression:** 0.5

### k

**Description:** Relaxation rate constant for sorption of B

**Type:** Formula Variable
**Unit:** 1/h

**Expression:** 10000

### Ke

**Description:** half velocity

**Type:** Constant Variable
**Unit:**

**Value:** 2.452503

**Standard Deviation:** 1

**Minimum:** 0.0005
Maximum: $1e+009$
Sensitivity Analysis: inactive
Parameter Estimation: inactive

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Type</th>
<th>Unit</th>
<th>Value</th>
<th>Standard Deviation</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Sensitivity Analysis</th>
<th>Parameter Estimation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kd</td>
<td>cell death coefficient</td>
<td>Constant Variable</td>
<td>m$^3$/kg</td>
<td>0.00058</td>
<td>1</td>
<td>0</td>
<td>10000</td>
<td>active</td>
<td>inactive</td>
</tr>
<tr>
<td>KF</td>
<td></td>
<td>Formula Variable</td>
<td></td>
<td>0.00025</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>kmc</td>
<td>Maximum specific Cr(VI) reduction rate coefficient</td>
<td>Constant Variable</td>
<td></td>
<td>1.53</td>
<td>1</td>
<td>0</td>
<td>100000</td>
<td>active</td>
<td>active</td>
</tr>
<tr>
<td>Qin</td>
<td></td>
<td>Formula Variable</td>
<td>m$^3$/h</td>
<td>0.001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Re</td>
<td>Inactivation capacity</td>
<td>Constant Variable</td>
<td>mg/mg</td>
<td>0.533764</td>
<td>1</td>
<td>0</td>
<td>100</td>
<td>active</td>
<td>inactive</td>
</tr>
<tr>
<td>rho_s</td>
<td>Density of solid material</td>
<td>Formula Variable</td>
<td>kg/m$^3$</td>
<td>2300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
S: Description: Adsorbed concentration
Type: Dyn. Surface State Var.
Unit: mg/kg
Relative Accuracy: 1e-006
Absolute Accuracy: 1e-009

Smax: Description: Formula Variable
Type: mg/kg
Unit: mg/kg
Expression: 0.00029

S_eq: Description: Isotherm
Type: Variable List Variable
Unit: mg/kg
Argument: calcnum
Interpolation Method: linear interpolation
Real-Variable Data Pairs (1 pairs):
0 S_eq_0

S_eq_0: Description: Isotherm for no sorption
Type: Formula Variable
Unit: mg/kg
Expression: Kd*C

S_eq_Freundlich: Description: Freundlich isotherm
Type: Formula Variable
Unit: mg/kg
Expression: if C>C_crit then KF*C^alpha else KF*C_crit^alpha*C/C_crit endif

S_eq_Langmuir: Description: Langmuir isotherm
Type: Formula Variable
Unit: mg/kg
Expression: Smax*C/(K+C)

S_eq_lin: Description: Linear isotherm
Type: Formula Variable
Unit: mg/kg
Expression: Kd*C

t: Description: Time
Type: Program Variable
Unit: d
Reference to: Time

theta: Description: Porosity
Type: Formula Variable
Unit:
Expression: 0.4

---
to: Description: initial time
Type: Constant Variable
Unit: days
Value: 20.356
Standard Deviation: 1
Minimum: 0
Maximum: 1000
Sensitivity Analysis: active
Parameter Estimation: inactive

---
X: Description: Biomass
Type: Formula Variable
Unit: mg/L
Expression: Xo+a/(1+(t/to) b)

---
Xo: Description: Concentration of viable cells at time t
Type: Constant Variable
Unit: mg/L
Value: 70.456994
Standard Deviation: 1
Minimum: 0
Maximum: 100000
Sensitivity Analysis: inactive
Parameter Estimation: inactive

---
Processes

Reduction: Description: Chromium(VI) Reduction
Type: Dynamic Process
Rate:
(K\(^{-1}\)\((Co-C5)/Co\))\(*kmc*C*(X)/(Kc+C )\)
Stoichiometry:
Variable : Stoichiometric Coefficient
C : -1

Sorption: Description:
Type: Dynamic Process
Rate: \(k*(S_{eq}-S)\)
Stoichiometry:
Variable : Stoichiometric Coefficient
C : \(-\rho_s*(1-\theta)/\theta\)
S : 1

---
Compartments

column: Description:
Type: Soil Column Compartment
Compartment Index: 0
Active Variables: C, S
Active Processes: Sorption, Reduction
Initial Conditions:
  Variable(Zone): Initial Condition
  C(Advective Zone): 0
Inflow: Qin
Loadings:
  Variable: Loading
  C: Qin*C_in
Lateral Inflow: 0
Start Coordinate: 0
End Coordinate: 1
Cross Section: A
Dispersion: D
Parallel Zones:
  Num. of Grid Pts: 52 (high resolution)
Accuracies:
  Rel. Acc. Q: 0.0001
  Abs. Acc. Q: 1e-006
  Rel. Acc. D: 1e-006
  Abs. Acc. D: 1e-006

Definitions of Calculations

calc_0: Description:
  Calculation Number: 0
  Initial Time: 0
  Initial State: given, made consistent
  Step Size: 0.02
  Num. Steps: 2300
  Status: active for simulation
         inactive for sensitivity analysis

Definitions of Parameter Estimation Calculations

fit1: Description:
  Calculation Number: 0
  Initial Time: 0
  Initial State: given, made consistent
  Status: active
  Fit Targets:
    Data: Variable
    (Compartment,Zone,Time/Space)
    Cmeas : C (column,Advective Zone,0)

Plot Definitions
plot: Description:
Abscissa: Time
Title: Break through curves
Abscissa Label: t [d]
Ordinate Label: C [mg/L]
Curves:
  Type : Variable
    [CalcNum,Comp.,Zone,Time/Space]
  Value : C [0,column,Advective Zone,1]
  Value : Cmeas [0,column,Advective Zone,0]
  Value : C_in_meas [0,column,Advective Zone,0]

---------------------------------------------------------------
X: Description:
Abscissa: Time
Title: Biomass
Abscissa Label:
Ordinate Label:
Curves:
  Type : Variable
    [CalcNum,Comp.,Zone,Time/Space]
  Value : X [0,column,Advective Zone,0]

Calculation Parameters

Numerical Parameters: Maximum Int. Step Size: 1
  Maximum Integrat. Order: 5
  Number of Codiagonals: 8
  Maximum Number of Steps: 1000

---------------------------------------------------------------
Fit Method: simplex
Max. Number of Iterat.: 100

Calculated States

Calc. Num. Num. States Comments
0    2301    Range of Times: 0 - 46
Figure B-1: Phylogenetic analysis of Gram-negative species of bacteria in the HR7 reactors at day 45. Possible Cr(VI) reducers were detected including Enterobacteriaceae, *Escherichia coli*, and *Citrobacter spp.* Bacteria originating from soil was detected including *Rhodobacter spp.* and *Alcaligenes spp.*
TARGET SITE AT THE DEFUNCT CHROME REFINERY, BRITS, NORTHWEST PROVINCE