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# Robust Dynamic Optimization via Relaxations of Implicit Integration Schemes

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Process Systems and Operations Research Laboratory

# Robust Dynamic Optimization

## Dynamic SIP Formulation

$$\Phi^* = \min_{\mathbf{u}} \Phi(\mathbf{u})$$ ← Objective

$$\text{s.t. } g(\mathbf{x}(\mathbf{u},\mathbf{p},\mathrm{t}_f),\mathbf{u},\mathbf{p}) \leq 0$$ ← Performance Constraint(s)

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}(\mathbf{u},\mathbf{p},\mathrm{t}),\mathbf{u},\mathbf{p})$$ ← Parametric ODEs

$$\mathbf{x}(\mathbf{u},\mathbf{p},\mathrm{t}_0) = \mathbf{x}_0(\mathbf{u},\mathbf{p})$$ ← Initial Condition

$$t \in I = [t_0, t_f], \forall \mathbf{p} \in P$$

**Motivation:**

- Determine adequate system performance under worst-case realization of uncertainty.
- Key for safety-critical systems and high-risk defect elimination.
- Prior work rely on heuristic approaches which lose strong guarantees [1,2].

## Assumptions

- The initial condition $\mathbf{x}_0: P \to D$ is *locally Lipschitz continuous* on $\mathrm{U} \times P$.
- The right hand side $\mathbf{f}$ is *n times continuously differentiable* on $\mathrm{U} \times D \times P$.


1. Puschke, Jennifer, et al. **Robust dynamic optimization of batch processes under parametric uncertainty: Utilizing approaches from semi-infinite programs.** *Computers & Chemical Engineering* 116 (2018): 253-267.
2. Puschke, Jennifer, and Alexander Mitsos. **Robust feasible control based on multi-stage eNMPC considering worst-case scenarios.** *Journal of Process Control* 69 (2018): 8-15.

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**Relatively general form (via reformulations):**

- Applicable to some semi-explicit index-1 DAEs
- Non-autonomous systems


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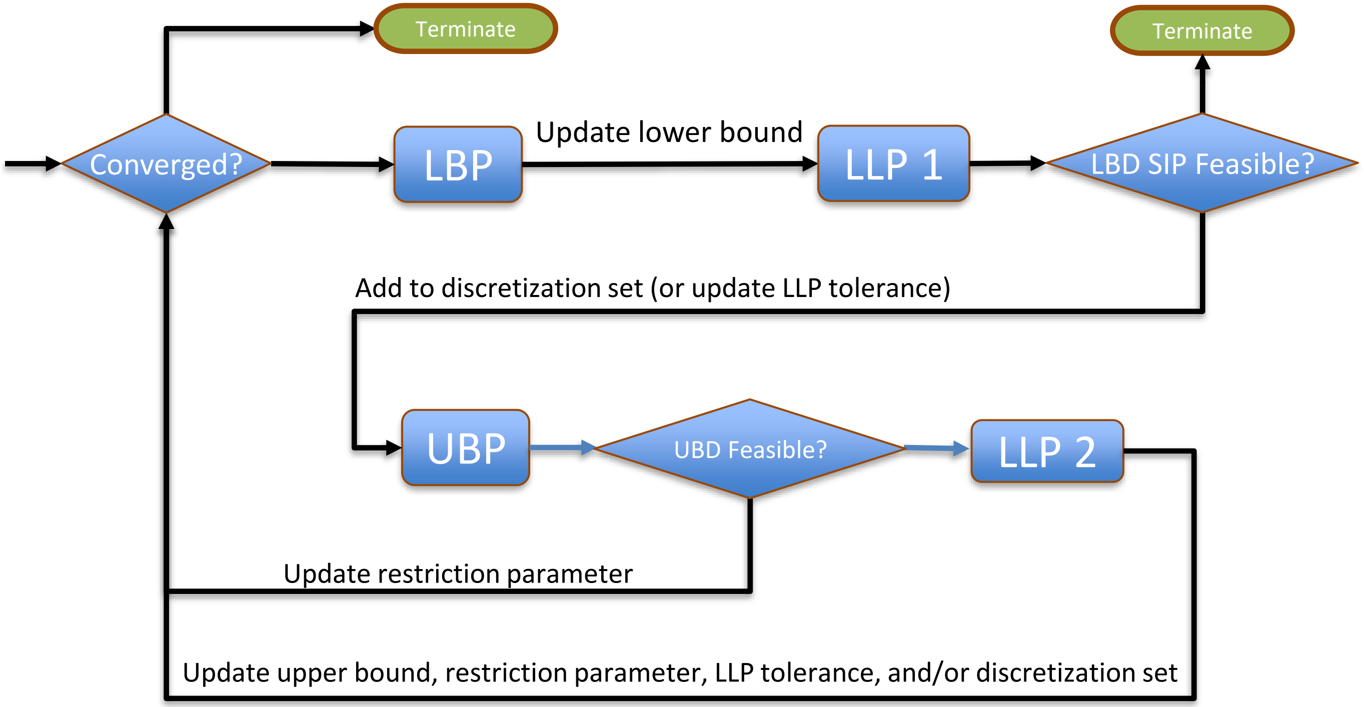
# Semi-infinite Programming

- One standard approach to solving SIP's lies in the discretization the uncertain set [3].
- Restriction-based upper bound incorporated in the SIPres algorithm for nonconvex SIP[4].
- SIPres provides a guaranteed convergence to a global optimal value under Slater-point constraint qualification.
- Adapted to use a hybrid approach which contains an oracle problem that further refines lower and upper bounds at each iteration with a single discretization set per SIP constraint (NOT PICTURED) [5].

## Overview of SIPres algorithm [1]





3. B. Bhattacharjee, P. Lemonidis, W.H. Green Jr, and P.I. Barton. **Global solution of semi-infinite programs.** *Math. Program*. 103 (2005), pp. 283–307.
4. Mitsos, Alexander. **Global optimization of semi-infinite programs via restriction of the right-hand side.** *Optimization* 60.10-11 (2011): 1291-1308.
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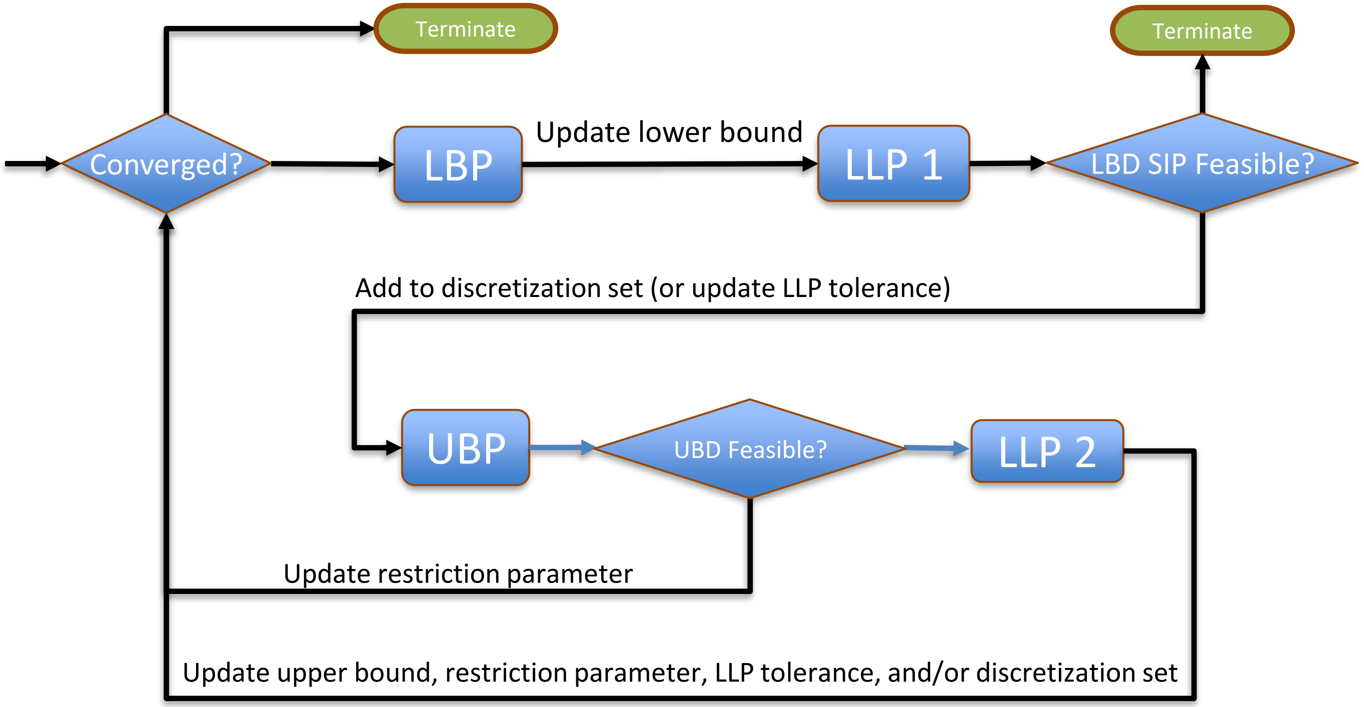


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# SIP Subproblems

LBP **Lower-Bounding Problem**

$$\Phi^{LBD} = \min_{\mathbf{u}} \Phi(\mathbf{u})$$

$$s.t.\ g\left(\mathbf{x}\left(\mathbf{u}, \bar{\mathbf{p}}, t_f\right), \mathbf{u}, \bar{\mathbf{p}}\right) \leq 0 \quad \forall \bar{\mathbf{p}} \in P^{disc}$$

$$\mathbf{u} \in U \subset \mathbb{R}^{n_u}$$

UBP **Upper-Bounding Problem**

$$\Phi^{UBD} = \min_{\mathbf{u}} \Phi(\mathbf{u})$$

$$s.t.\ g\left(\mathbf{x}\left(\mathbf{u}, \bar{\mathbf{p}}, t_f\right), \mathbf{u}, \bar{\mathbf{p}}\right) \leq -\epsilon_g \quad \forall \bar{\mathbf{p}} \in P^{disc}$$

$$\mathbf{u} \in U \subset \mathbb{R}^{n_u}$$

LLP **Lower-Level Problem**

$$\Phi^{LLP} = \max_{\mathbf{p}} g\left(\mathbf{x}\left(\bar{\mathbf{u}}, \mathbf{p}, t_f\right), \bar{\mathbf{u}}, \mathbf{p}\right)$$

$$s.t.\ \mathbf{p} \in P \subset \mathbb{R}^{n_p}$$

RES* **Restriction Problem**

$$-\eta^* = \min_{\eta, \mathbf{u}} -\eta$$

$$s.t.\ \Phi(\mathbf{u}) - \Phi^{RES} \leq 0$$

$$g\left(\mathbf{x}\left(\mathbf{u}, \bar{\mathbf{p}}, t_f\right), \mathbf{u}, \bar{\mathbf{p}}\right) \leq -\eta \quad \forall \bar{\mathbf{p}} \in P^{disc}$$

$$\mathbf{u} \in U \subset \mathbb{R}^{n_u}$$


4. Mitsos, Alexander. **Global optimization of semi-infinite programs via restriction of the right-hand side.** *Optimization* 60.10-11 (2011): 1291-1308.
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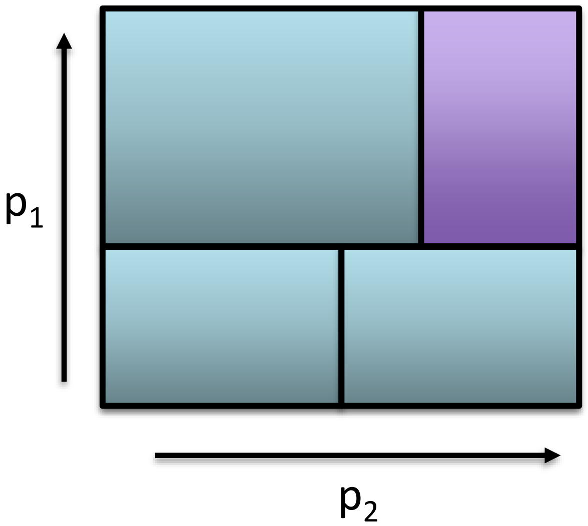
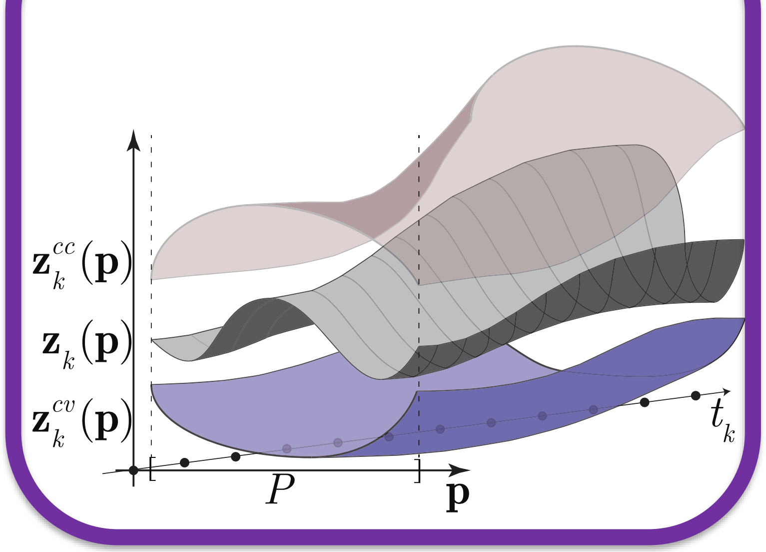
# Global Dynamic Optimization

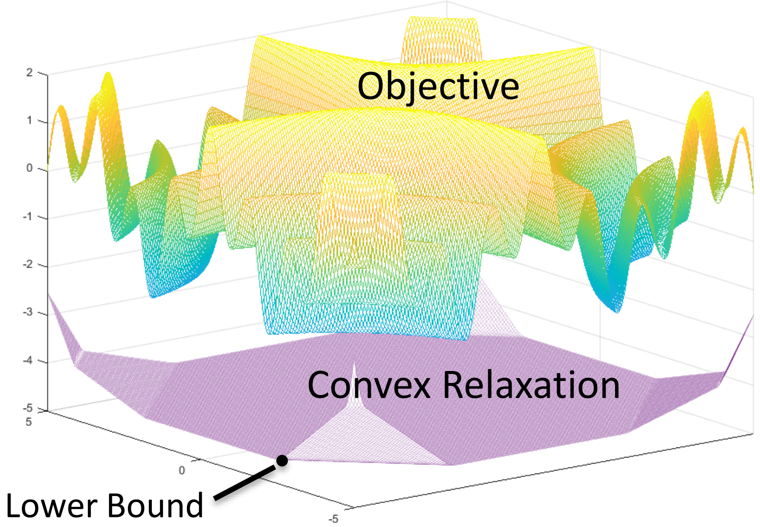
*(Selection of Node)*




*(Relaxation of Intermediate Values)*[5]




*(Relaxation of Objective and Constraints)*




McCormick Operator Arithmetic[7,8,9]


6. Wilhelm, ME; Le, AV; and Stuber. MD. **Global Optimization of Stiff Dynamical Systems.** *AIChE Journal: Futures Issue,* 65 (12), *2019*
7. Mitsos, A, et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
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# Reduced-Space Relaxations

## Relax-then-Discretize

$$\dot{\mathbf{x}}^{cv}(t,\mathbf{p}) = \mathbf{f}^{cv}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cv}(t_0,\mathbf{p}) = \mathbf{x}_0^{cv}(\mathbf{p})$$
$$\dot{\mathbf{x}}^{cc}(t,\mathbf{p}) = \mathbf{f}^{cc}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cc}(t_0,\mathbf{p}) = \mathbf{x}_0^{cc}(\mathbf{p})$$

- Development of interval-based differential inequality [10,11]
- Less expansive convex/concave relaxations as well as tighter interval bounds [12,13,14]
- Adaptation of these methods to semi-explicit index-one differential-algebraic systems of equations DAEs [15,16,17]
- Methods of tightening state relaxations by exploiting model redundancy and nonlinear invariants [18,19].

## Discretize-then-Relax

$$\mathbf{x}(\tau_{q+1},\mathbf{p}) \in \underbrace{\mathbf{x}(\tau_q,\mathbf{p}) + \sum_{j=1}^{p} \frac{h^j}{j!}\mathbf{f}^{(j)}(\mathbf{x}(\tau_q,\mathbf{p}),\mathbf{p})}_{\text{Taylor Series}} + \underbrace{\frac{h^{p+1}}{(p+1)!}\mathbf{f}^{(p+1)}(\mathrm{X}(\tau_q),\mathrm{P})}_{\text{Remainder Bound}}$$

- First introduced by Moore [20] based on simple existence test.
- Generalized to two step methods consisting of an existence and uniqueness test and subsequent contraction [21,22].
- Discretize-and-relax approaches with McCormick relaxations [23]
- Taylor-Interval [24], Taylor-McCormick [25] models, and Taylor-Ellipsoid [26] models were introduced which enclosure the remainder term using different set-valued arithmetic.


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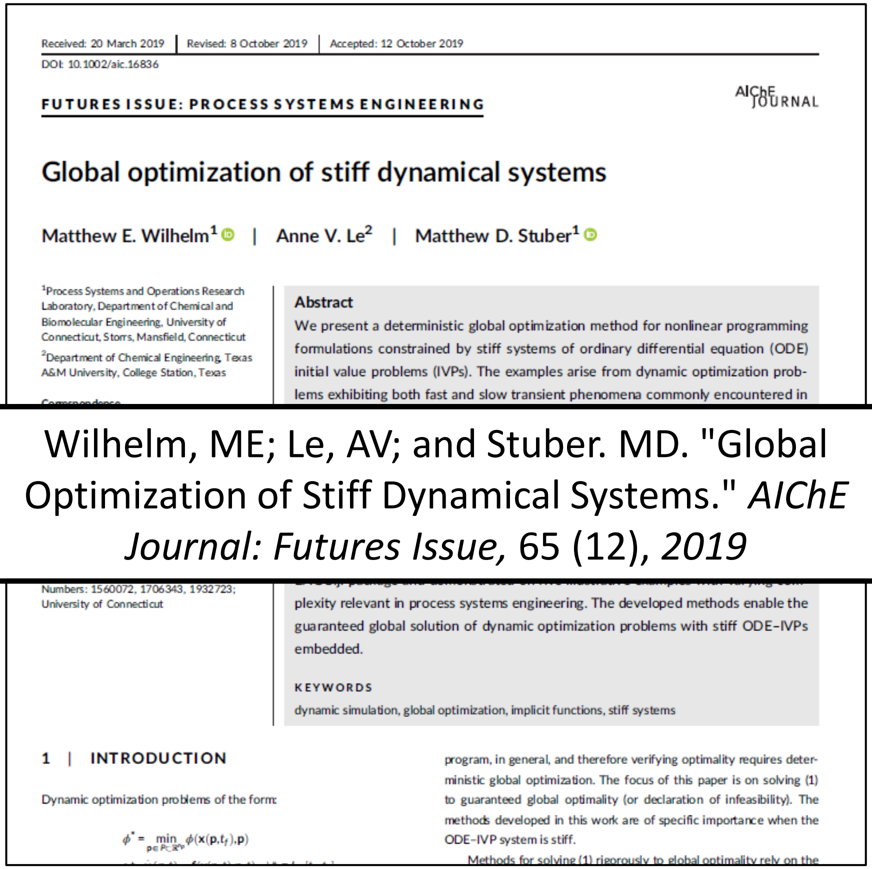
# Prior Work: Stiff Systems and Global Optimization



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## Global optimization of stiff dynamical systems

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**Abstract**
We present a deterministic global optimization method for nonlinear programming formulations constrained by stiff systems of ordinary differential equation (ODE) initial value problems (IVPs). The examples arise from dynamic optimization problems exhibiting both fast and slow transient phenomena commonly encountered in ... plexity relevant in process systems engineering. The developed methods enable the guaranteed global solution of dynamic optimization problems with stiff ODE–IVPs embedded.

Numbers: 1560072, 1706343, 1932723; University of Connecticut

KEYWORDS
dynamic simulation, global optimization, implicit functions, stiff systems

1 | INTRODUCTION

Dynamic optimization problems of the form:

$$\phi^* = \min_{p \in P \subset \mathbb{R}^{n_p}} \phi(\mathbf{x}(\mathbf{p}, t_f), \mathbf{p})$$

program, in general, and therefore verifying optimality requires deterministic global optimization. The focus of this paper is on solving (1) to guaranteed global optimality (or declaration of infeasibility). The methods developed in this work are of specific importance when the ODE–IVP system is stiff.

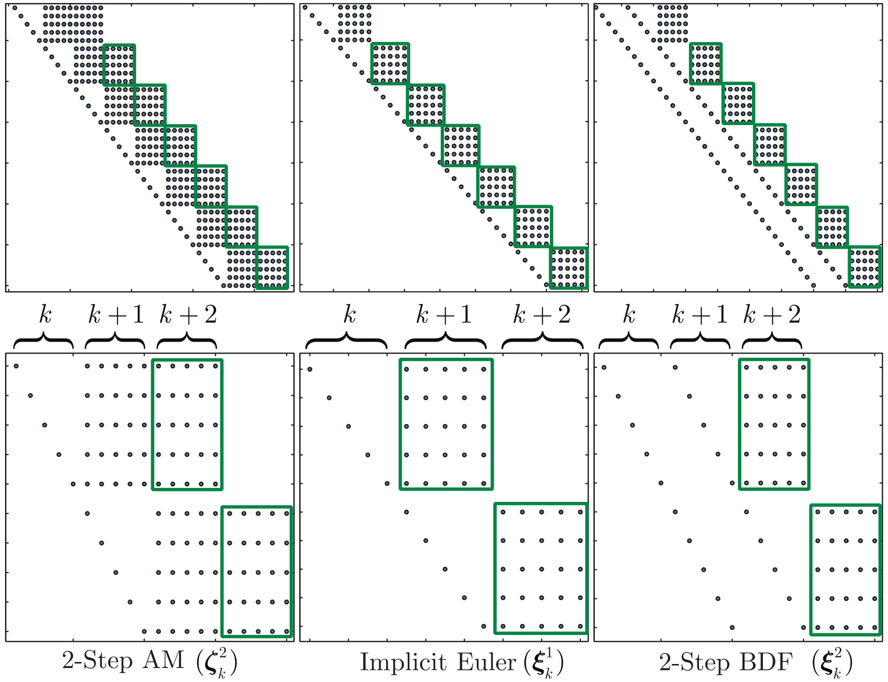
Methods for solving (1) rigorously to global optimality rely on the

Wilhelm, ME; Le, AV; and Stuber. MD. "Global Optimization of Stiff Dynamical Systems." *AIChE Journal: Futures Issue*, 65 (12), *2019*

(*Implicit Euler*[27,28]) $\boldsymbol{\xi}_k^1 \equiv \hat{\mathbf{z}}_{k+1} - \hat{\mathbf{z}}_k - \Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p})$

(*Two-step Adam-Moulton*[27,28]) $\boldsymbol{\xi}_k^2 \equiv \hat{\mathbf{z}}_{k+2} - \frac{4}{3}\hat{\mathbf{z}}_{k+1} + \frac{1}{3}\hat{\mathbf{z}}_k - \frac{2}{3}\Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p})$

(*Two-step BDF*[27,28]) $\boldsymbol{\zeta}_k^2 \equiv \hat{\mathbf{z}}_{k+2} - \hat{\mathbf{z}}_{k+1} - \frac{1}{2}\Delta t\left(\mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p}) + \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p})\right)$

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28. Hairer E, Wanner G. **Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems**. *Springer, Heidelberg*; 1991.

# Integration Scheme

- Discretize-then-relax algorithm employed.
- Higher-order existence test used[22,29].
- Local error per unit step (LEPUS) adaptive step-size control scheme used[30].
- **Step 1:** Determines step-size and state relaxations for the **entire** step ($t \in [t_j, t_{j+1}]$)[22,30].
- **Step 2:** Refines state relaxations at new time ($t = t_{j+1}$).


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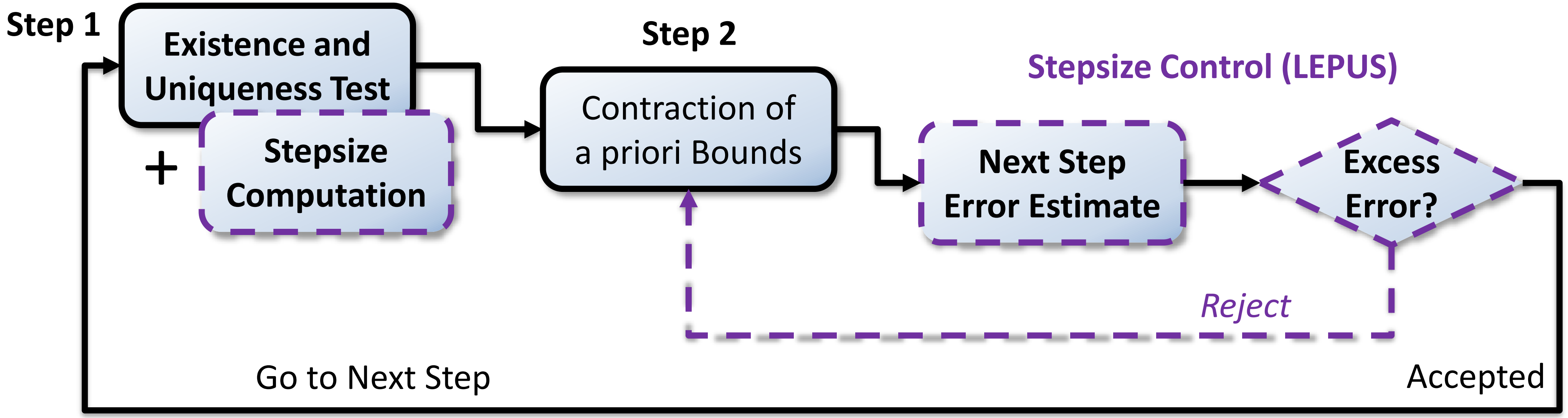

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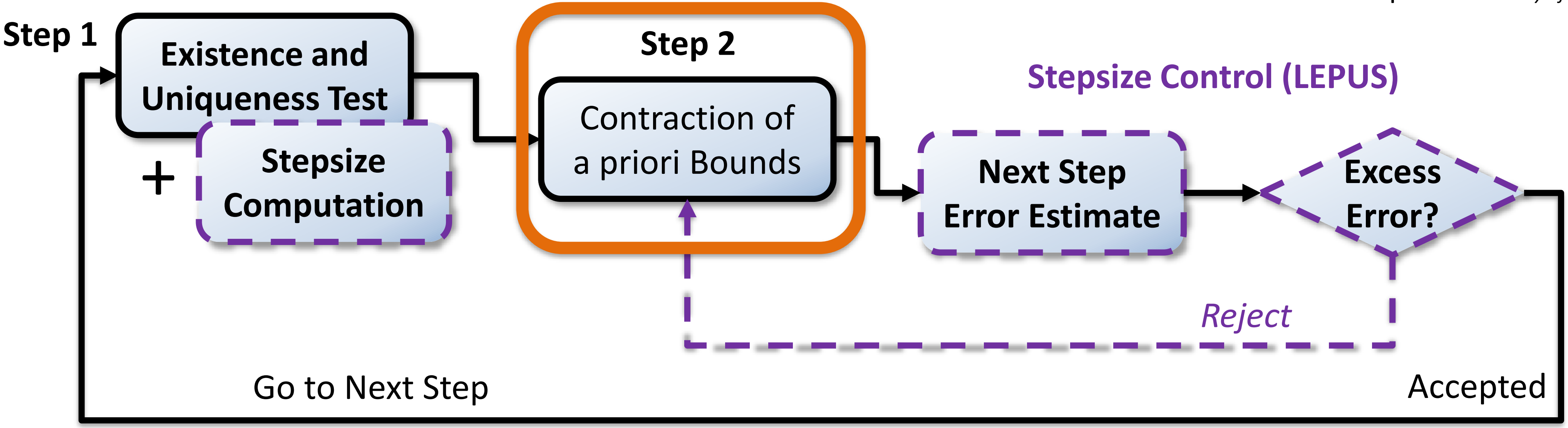

# Adams-Moulton: Pointwise

## Adams-Moulton Method[27,28]

$$\mathbf{x}(\mathbf{p}, t_k) = \mathbf{x}(\mathbf{p}, t_{k-1}) + h\sum_{j=0}^{n} \bar{\beta}_{jn}\, \mathbf{f}\big(\mathbf{x}(\mathbf{p}, t_{k-j}), \mathbf{p}\big)$$

$$t_{k-n}, \ldots, t_k \in [t_{k-n}, t_k]$$

## Truncation Error[31] ($\tau$)

$$\tau(\mathbf{p}, \bar{\eta}) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{x}^{(n+2)}(\mathbf{p}, \bar{\eta})$$

$$\tau(\mathbf{p}, \bar{\eta}) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{f}^{(n+1)}(\mathbf{x}(\mathbf{p}, \bar{\eta}), \mathbf{p})$$

$$\exists \bar{\eta} \in [t_{k-n}, t_k]$$

## Nonlinear System of Equations

$$\mathbf{h}(\mathbf{z}(\mathbf{p}), \mathbf{p}) = \mathbf{x}(\mathbf{p}, t_k) - \mathbf{x}(\mathbf{p}, t_{k-1}) - h\sum_{j=0}^{n} \bar{\beta}_{jn}\, \mathbf{f}\big(\mathbf{x}(\mathbf{p}, t_{k-j}), \mathbf{p}\big) = \mathbf{0}$$

$$\mathbf{z}(\mathbf{p}) = [\mathbf{x}(\mathbf{p}, t_k); \mathbf{x}(\mathbf{p}, t_{k-1}); \ldots; \mathbf{x}(\mathbf{p}, t_{k-n})]$$

- A n-step Adams-Moulton arises from a Lagrange interpolation polynomial appropriating the solution at n+1 points, $t_{k-n}, \ldots, t_k$, in the time interval $[t_{k-n}, t_k]$[27,28].
- These methods exhibit preferable regions of stability for stiff systems when compared with many explicit methods[27,28].


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# Adams-Moulton: Pointwise

## Adams-Moulton Method[27,28]

## Truncation Error[31] ($\tau$)

$$) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{x}^{(n+2)}(\mathbf{p},\bar{\eta})$$

$$) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{f}^{(n+1)}(\mathbf{x}(\mathbf{p},\bar{\eta}),\mathbf{p})$$

$$[t_{k-n}, t_k]$$

- Compute relaxation for **truncation error** in standard manner
- Compute relaxation of implicit function using approach of Stuber et al. 2015[32] and Wilhelm et al. 2019[6].

$$\mathbf{h}(\mathbf{z}(\mathbf{p}),\mathbf{p}) = \mathbf{x}(\mathbf{p},t_k) - \mathbf{x}(\mathbf{p},t_{k-1}) - h\sum_{j=0}^{n}\bar{\beta}_{jn}\,\mathbf{f}\big(\mathbf{x}(\mathbf{p},t_{k-j}),\mathbf{p}\big) = 0$$

*Nonlinear System of Equations (Defining implicit function)*

$$\mathbf{h}(\mathbf{z}(\mathbf{p}),\mathbf{p}) = \mathbf{x}(\mathbf{p},t_k) - \mathbf{x}(\mathbf{p},t_{k-1}) - h\sum_{j=0}^{n}\bar{\beta}_{jn}\,\mathbf{f}\big(\mathbf{x}(\mathbf{p},t_{k-j}),\mathbf{p}\big) + \tau(\mathbf{p},\bar{\eta}) = \mathbf{0}$$

$$\mathbf{z}(\mathbf{p}) = [\mathbf{x}(\mathbf{p},t_k); \mathbf{x}(\mathbf{p},t_{k-1}); \ldots; \mathbf{x}(\mathbf{p},t_{k-n})]$$


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...Malgorzata A. Jankowska, and ...n interval predictor- ...*Numerical Algorithms* 75.3

# Adams-Moulton: Mean Value Form

**Mean value form** of n-step Adams-Moulton method

$$\mathbf{x}_k = \underbrace{\hat{\mathbf{x}}_{k-1} + h\sum_{j=0}^{n}\bar{\beta}_{jn}\,\mathbf{f}\left(\hat{\mathbf{x}}_{k-j},\hat{\mathbf{p}}\right) + \overset{\text{truncation error}}{\boxed{\mathbf{R}_k(\mathbf{p})}}}_{\mathbf{D}_k(\mathbf{p})} + \underbrace{\sum_{j=0}^{n} h\bar{\beta}_{jn}\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\left(\boldsymbol{\mu}_{k-j}(\mathbf{p}),\boldsymbol{\rho}(\mathbf{p})\right)}_{\mathbf{J}_p^k(\mathbf{p})}(\mathbf{p}-\hat{\mathbf{p}})$$

$$+\underbrace{\left(\mathbf{I} + h\bar{\beta}_{1n}\frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}}\left(\boldsymbol{\mu}_{k-1}(\mathbf{p}),\boldsymbol{\rho}(\mathbf{p})\right)\right)}_{\mathbf{I}+\mathbf{J}_x^{k-1}(\mathbf{p})}(\mathbf{x}_{k-1}-\hat{\mathbf{x}}_{k-1}) + \sum_{\substack{j=0\\ j\neq 1}}^{n} h\underbrace{\bar{\beta}_{jn}\frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-j}}\left(\boldsymbol{\mu}_{k-j}(\mathbf{p}),\boldsymbol{\rho}(\mathbf{p})\right)}_{\mathbf{J}_x^{k-j}(\mathbf{p})}(\mathbf{x}_{k-j}-\hat{\mathbf{x}}_{k-j})$$

Were we define $\boldsymbol{\mu}_k$ and $\boldsymbol{\rho}$ as below

$$\boldsymbol{\mu}_k(\mathbf{p}) = \eta(\mathbf{x}_k - \hat{\mathbf{x}}_k) + \hat{\mathbf{x}}_k$$

$$\boldsymbol{\rho}(\mathbf{p}) = \eta(\mathbf{p} - \hat{\mathbf{p}}) + \mathbf{p}$$

$$\eta \in [0,1]$$

**Truncation error** notation and form

$$\mathbf{R}_k(\mathbf{p}) = h^{n+2}\,\bar{\gamma}_{n+1}\mathbf{f}^{(n+1)}(\tilde{\mathbf{x}}(\mathbf{p},t_{k-n};t_k),\mathbf{p})$$

# Adams-Moulton: Interval

**Mean value form** of n-step Adams-Moulton method

$$\mathbf{x}_k = \mathbf{D}_k(\mathbf{p}) + \mathbf{J}_p^k(\mathbf{p})(\mathbf{p}-\hat{\mathbf{p}}) + \left(\mathbf{I}+\mathbf{J}_x^{k-1}(\mathbf{x}_{k-1},\mathbf{p})\right)(\mathbf{x}_{k-1}-\hat{\mathbf{x}}_{k-1}) + \sum_{\substack{j=0\\ j\neq 1}}^{n} \mathbf{J}_x^{k-j}(\mathbf{x}_{k-j},\mathbf{p})(\mathbf{x}_{k-j}-\hat{\mathbf{x}}_{k-j})$$

**Interval bounds** of n-step Adams-Moulton method

$$\mathbf{X}_k = \mathrm{D}_k(\mathrm{P}) + \mathbf{J}_p^k(\mathrm{P})(\mathrm{P}-\hat{\mathbf{p}}) + \left(\mathbf{I}+\mathbf{J}_x^{k-1}(X_{k-1},\mathrm{P})\right)(X_{k-1}-\hat{\mathbf{x}}_{k-1}) + \sum_{j=2}^{n} \mathbf{J}_x^{k-j}(X_{k-j},\mathrm{P})(X_{k-j}-\hat{\mathbf{x}}_{k-j}) + \mathbf{J}_x^k(X_k,\mathrm{P})(X_k^0-\mathbf{x}_k^{\mathbf{0}})$$

- ❑ Uncertain set is propagated as a parallelepiped[22,33].
- ❑ Namely, that there exist $\mathbf{A}_k \in \mathbb{R}^{n_x \times n_x}$ and $\boldsymbol{\delta}_k \in \Delta_k$ such that $x_k(\mathbf{p}) - \hat{x}_k = \mathbf{A}_k\boldsymbol{\delta}_k \in \mathbf{A}_k\Delta_k$.

$$X_k := \left( \mathrm{D}_k(\mathrm{P}) + \mathbf{J}_p^k(\mathrm{P})(\mathrm{P}-\hat{\mathbf{p}}) + \left(\mathbf{I}+\mathbf{J}_x^{k-1}(\mathrm{P})\right)\mathbf{A}_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} \mathbf{J}_x^{k-j}(X_{k-j},\mathrm{P})\mathbf{A}_{k-j}\Delta_{k-j} + \mathbf{J}_x^k(X_k^0,\mathrm{P})(X_k^0-\hat{\mathbf{x}}_k^{\mathbf{0}}) \right) \cap X_k^0$$


22. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.

33. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

# Adams-Moulton: Interval

**Mean value form** of n-step Adams-Moulton method

$$\mathbf{x}_{\mathrm{k}} = \mathbf{D}_k(\mathbf{p}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{p})(\mathbf{p} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathbf{x}_{\mathrm{k-1}}, \mathbf{p})\right)(\mathbf{x}_{\mathrm{k-1}} - \hat{\mathbf{x}}_{\mathrm{k-1}}) + \sum_{\substack{j=0 \\ j\neq 1}}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathbf{x}_{\mathrm{k-j}}, \mathbf{p})(\mathbf{x}_{\mathrm{k-j}} - \hat{\mathbf{x}}_{\mathrm{k-j}})$$

**Interval bounds** of n-step Adams-Moulton method

$$\mathbf{X}_{\mathrm{k}} = \mathbf{D}_k(\mathrm{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathrm{P})(\mathrm{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathrm{X}_{k-1}, \mathrm{P})\right)(\mathrm{X}_{k-1} - \hat{\mathbf{x}}_{\mathrm{k-1}}) + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathrm{X}_{k-j}, \mathrm{P})(\mathrm{X}_{k-j} - \hat{\mathbf{x}}_{\mathrm{k-j}}) + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathrm{X}_k, \mathrm{P})(\mathrm{X}_k^0 - \mathbf{x}_{\boldsymbol{k}}^{\mathbf{0}})$$

- Uncertain set is propagated as a parallelepiped[22,33].
- Namely, that there exist $\mathbf{A}_{\mathrm{k}} \in \mathbb{R}^{n_x \times n_x}$ and $\boldsymbol{\delta}_{\mathrm{k}} \in \Delta_{\mathrm{k}}$ such that $\mathrm{x}_{\mathrm{k}}(\mathbf{p}) - \hat{\mathrm{x}}_{\mathrm{k}} = \mathbf{A}_{\mathrm{k}}\boldsymbol{\delta}_{\mathrm{k}} \in \mathbf{A}_{\mathrm{k}}\Delta_{\mathrm{k}}$.

$$\mathrm{X}_k := \left( \mathrm{D}_k(\mathrm{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathrm{P})(\mathrm{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathrm{P})\right)\mathbf{A}_{\mathrm{k-1}}\Delta_{\mathrm{k-1}} + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathrm{X}_{k-j}, \mathrm{P})\mathbf{A}_{\mathrm{k-j}}\Delta_{\mathrm{k-j}} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathrm{X}_k^{\mathbf{0}}, \mathrm{P})(\mathrm{X}_k^0 - \hat{\mathbf{x}}_{\boldsymbol{k}}^{\mathbf{0}}) \right) \cap X_k^0$$


22. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.

33. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

# Adams-Moulton: Interval

## Initialization for parallelepiped[22,33]

$$\mathbf{A}_0 = \mathbf{I} \qquad \Delta_0 = \mathrm{X}_0 - \hat{\mathbf{x}}_0$$

## Parallelepiped update at step k


22. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
33. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.


$\mathbf{A}_\mathrm{k}$ update given by taking to be orthogonal matrix Q of QR decomposition of $\mathrm{mid}(\mathbf{J}_\mathrm{x}^\mathrm{k}\mathbf{A}_{\mathrm{k}-1})$[22,33]

$$\Delta_\mathrm{k} = \mathbf{A}_\mathrm{k}^{-1}\left(\mathrm{D}_k(\mathrm{P}) + \mathbf{J}_\mathrm{p}^\mathrm{k}(\mathrm{P})(\mathrm{P}-\hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_\mathrm{x}^{\mathrm{k}-1}(\mathrm{P})\right)\mathbf{A}_{\mathrm{k}-1}\Delta_{\mathrm{k}-1} + \sum_{j=2}^{n}\mathbf{J}_\mathrm{x}^{\mathrm{k}-\mathrm{j}}(\mathrm{X}_k,\mathrm{P})\mathbf{A}_{\mathrm{k}-\mathrm{j}}\Delta_{\mathrm{k}-\mathrm{j}} + \mathbf{J}_\mathrm{x}^\mathrm{k}(\mathrm{X}_k,\mathrm{P})(\mathrm{X}_k - \hat{\mathbf{x}}_\mathrm{k})\right)$$

## Bound truncation error via partition

$$\mathrm{R}_k(\mathrm{P}) \equiv \mathrm{h}^{\mathrm{n}+2}\,\overline{\gamma}_{\mathrm{n}+1}\bigcup_{j=0}^{n}\mathrm{F}^{(\mathrm{n}+1)}\left(\widetilde{\mathrm{X}}_{k-j},\mathrm{P}\right) \subseteq \mathrm{h}^{\mathrm{n}+2}\,\overline{\gamma}_{\mathrm{n}+1}\mathrm{F}^{(\mathrm{n}+1)}\left(\bigcup_{j=0}^{n}\widetilde{\mathrm{X}}_{k-\mathrm{j}},\mathrm{P}\right)$$

# Adams-Moulton: Interval

**Initialization for parallelepiped**[22,33]

$$\mathbf{A}_0 = \mathbf{I} \qquad \Delta_0 = \mathbf{X}_0 - \hat{\mathbf{x}}_0$$

**Parallelepiped update at step k**


22. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
33. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.


$\mathbf{A}_k$ update given by taking to be orthogonal matrix Q of QR decomposition of $\mathrm{mid}(\mathbf{J}_x^k \mathbf{A}_{k-1})$[22,33]

$$\Delta_k = \mathbf{A}_k^{-1}\left(D_k(P) + \mathbf{J}_p^k(P)(P - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_x^{k-1}(P)\right)\mathbf{A}_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} \mathbf{J}_x^{k-j}(X_k, P)\mathbf{A}_{k-j}\Delta_{k-j} + \mathbf{J}_x^k(X_k, P)(X_k - \hat{\mathbf{x}}_k)\right)$$

**Bound truncation error via partition**

$$R_k(P) \equiv h^{n+2}\bar{\gamma}_{n+1}\bigcup_{j=0}^{n} F^{(n+1)}(\tilde{X}_{k-j}, P) \subseteq h^{n+2}\bar{\gamma}_{n+1}F^{(n+1)}\left(\bigcup_{j=0}^{n}\tilde{X}_{k-j}, P\right)$$

# Adams-Moulton: Relaxation

**Interval update** of n-step Adams-Moulton method

$$\mathrm{X}_k := \left( \mathrm{D}_k(\mathrm{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathrm{P})(\mathrm{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-1}(\mathrm{P})\right) \mathbf{A}_{\mathrm{k}-1}\Delta_{\mathrm{k}-1} + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-\mathrm{j}}\left(\mathrm{X}_{\mathrm{k}-j}, \mathrm{P}\right)\mathbf{A}_{\mathrm{k}-\mathrm{j}}\Delta_{\mathrm{k}-\mathrm{j}} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}\left(\mathrm{X}_k^0, \mathrm{P}\right)\left(\mathrm{X}_k^0 - \mathbf{x}_{\boldsymbol{k}}^{\mathbf{0}}\right) \right) \cap \mathrm{X}_k^0$$

**Convex/concave relaxation update** of n-step Adams-Moulton method

Let $\{\mathbf{g}^{\mathbf{cv}}, \mathbf{g}^{\mathbf{cc}}\}(\mathbf{p})$ denote the tuple of convex and concave relaxations of $\mathbf{g}$ on P evaluated at $\mathbf{p} \in \mathrm{P}$:

$$\{\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}\}(\mathbf{p}) := \{\mathbf{D}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{D}_{\mathbf{k}}^{\mathbf{cc}}\}(\mathbf{p}) + \{\mathbf{J}_{\mathbf{p}}^{\mathbf{k,cv}}, \mathbf{J}_{\mathbf{p}}^{\mathbf{k,cc}}\}(\mathbf{p})(\mathbf{p} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \{\mathbf{J}_{\mathbf{x}}^{\mathbf{k-1,cv}}, \mathbf{J}_{\mathbf{x}}^{\mathbf{k-1,cc}}\}(\mathbf{p})\right) \otimes \mathbf{A}_{\mathrm{k}-1}\{\Delta_{\mathrm{k}-1}^{\mathrm{cv}}, \Delta_{\mathrm{k}-1}^{\mathrm{cc}}\}(\mathbf{p})$$

$$+ \sum_{j=2}^{n} \left\{\mathbf{J}_{\mathbf{x}}^{\mathbf{k-j,cv}}, \mathbf{J}_{\mathbf{x}}^{\mathbf{k-j,cc}}\right\}(\mathbf{p})\mathbf{A}_{\mathrm{k}-\mathrm{j}}\{\Delta_{\mathrm{k}-1}^{\mathrm{cv}}, \Delta_{\mathrm{k}-1}^{\mathrm{cc}}\}(\mathbf{p})\,\{\mathbf{J}_{\mathbf{x}}^{\mathbf{k,cv}}, \mathbf{J}_{\mathbf{x}}^{\mathbf{k,cc}}\}(\mathbf{p})\left(\{\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cv}}, \mathbf{x}_{\mathbf{k}}^{\mathbf{0,cc}}\}(\mathbf{p}) - \hat{\mathbf{x}}_{\boldsymbol{k}}^{\mathbf{0}}\right)$$

$$\{\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}\}(\mathbf{p}) := \mathrm{intersect}\left(\{\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}\}(\mathbf{p}), \mathrm{X}_{\mathrm{k}}^{0}\right)$$

# Adams-Moulton: Relaxation

## Generalization of Union:

Compute union $\left(\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p}), \{\mathbf{x}_k^{0,cv}, \mathbf{x}_k^{0,cc}\}(\mathbf{p})\right)$ and update $\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p})$ as follows:

*Step 1:* $\{\boldsymbol{\varphi}_l^{cv}, \boldsymbol{\varphi}_l^{cc}\}(\mathbf{p}) \longleftarrow \min(\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p}), \{\mathbf{x}_k^{0,cv}, \mathbf{x}_k^{0,cc}\}(\mathbf{p}))$

*Step 2:* $\{\boldsymbol{\varphi}_u^{cv}, \boldsymbol{\varphi}_u^{cc}\}(\mathbf{p}) \longleftarrow \max(\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p}), \{\mathbf{x}_k^{0,cv}, \mathbf{x}_k^{0,cc}\}(\mathbf{p}))$

*Step 3:* $\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p}) \longleftarrow : \{\boldsymbol{\varphi}_l^{cv}, \boldsymbol{\varphi}_u^{cc}\}(\mathbf{p})$

Pairwise composite relaxations of min/max evaluated by McCormick arithmetic

## Bound truncation error via partition

$$\{\mathbf{R}_k^{cv}, \mathbf{R}_k^{cc}\}(\mathbf{p}) = h^{n+2}\,\bar{\gamma}_{n+1}\text{union}\left(\text{union}\left(\mathbf{f}^{(n+1)}(\{\mathbf{x}_k^{cv}, \mathbf{x}_k^{cc}\}(\mathbf{p}), \mathbf{p}), \ldots\right), \mathbf{f}^{(n+1)}(\{\mathbf{x}_{k-n}^{cv}, \mathbf{x}_{k-n}^{cc}\}(\mathbf{p}), \mathbf{p})\right)$$

## Subgradient-based tightening of state bounds:

Update interval bounds at **k** by using interval extension of affine relaxations compute at $p_{ref}$ if an improvement[14].

22. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.

# Implementation

**Customizable Global and Robust Optimization Routines**

EAGO

***Implicit Linear Multistep Relaxations***

**EAGODynamicOptimizer.jl**


34. Wilhelm, M. E., and M. D. Stuber. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software* (2020): 1-26.
35. Bezanson, Jeff, et al. **Julia: A fresh approach to numerical computing.** *SIAM review* 59.1 (2017): 65-98.

# Implementation

## Customizable Global and Robust Optimization Routines

EAGO

*Implicit Linear Multistep Relaxations*

**EAGODynamicOptimizer.jl**

## Abstract Layer for Dynamic Problems

**DynamicBounds.jl**

- **DynamicBounds.jl** – Wrapper for dependent modules
- **DynamicBoundsBase.jl** – Abstraction Layer
- **DynamicBoundspODEsDiscrete.jl**
  – Discrete time approaches
- **DynamicBoundspODEsIneq.jl**
  -- Continuous time approaches


34. Wilhelm, M. E., **DynamicBounds.jl**, (2020), GitHub repository, https://github.com/PSORLab/DynamicBounds.jl
35. Wilhelm, M. E., **EAGODynamicOptimizer.jl**, (2020), GitHub repository, https://github.com/PSORLab/EAGODynamicOptimizer.jl
36. Wilhelm, M. E., **McCormick.jl**, (2020), GitHub repository, https://github.com/PSORLab/McCormick.jl
37. Wilhelm, M. E., and M. D. Stuber. **EAGO. jl: easy advanced global optimization in Julia.** *Optimization Methods and Software* (2020): 1-26.
38. Bezanson, Jeff, et al. **Julia: A fresh approach to numerical computing.** *SIAM review* 59.1 (2017): 65-98.

# Implementation

**Customizable Global and Robust Optimization Routines**

**Abstract Layer for Dynamic Problems**

**unds.jl**

dependent modules
tion Layer

***Implicit***
***Multistep F***

- **IntervalArithmetic.jl** for validated interval calculations.
- Relaxations from McCormick.jl[36] submodule of **EAGO.jl**[37].
- All simulations run on single thread of Intel Xeon E3-1270 v5 3.60/4.00GHz processor with 16GM ECC RAM, Ubuntu 18.04LTS using Julia v1.5.1[38]. Intel MKL 2019 (Update 2) for BLAS/LAPACK.


34. Wilhelm, M. E., **DynamicBounds.jl**, (2020), GitHub repository, https://github.com/PSORLab/DynamicBounds.jl
35. Wilhelm, M. E., **EAGODynamicOptimizer.jl**, (2020), GitHub repository, https://github.com/PSORLab/EAGODynamicOptimizer.jl
36. Wilhelm, M. E., **McCormick.jl**, (2020), GitHub repository, https://github.com/PSORLab/McCormick.jl
37. Wilhelm, M. E., and M. D. Stuber. **EAGO. jl: easy advanced global optimization in Julia.** *Optimization Methods and Software* (2020): 1-26.
38. Bezanson, Jeff, et al. **Julia: A fresh approach to numerical computing.** *SIAM review* 59.1 (2017): 65-98.

# Kinetic Problem - Formulation

*(Objective Function)*

$$\Phi^* = \min_{\boldsymbol{p}\in P} \sum_{i=1}^{n} \left(\mathrm{I}^i - \mathrm{I}^i_{\mathrm{data}}\right)^2$$

$$s.t. \quad \mathrm{I}^i = x_A^i + \frac{2}{21} x_B^i + \frac{2}{21} x_D^i$$

*(Description of Problem)*

- Fit the rate constants ($k_{2f}$, $k_{3f}$, $k_4$) of oxygen addition to cyclohexadienyl radicals to data. [39]
- First addressed by global by Singer et al.[40]
- Explicit Euler form solved by Mitsos[3]
- Implicit Euler form addressed in Stuber[32]
- Two-step PILMS forms addressed in Wilhelm[6]

*(pODE IVP)*

$$\dot{\mathrm{x}}_A = \mathrm{k}_1\mathrm{x}_Z\mathrm{x}_Y - \mathrm{c}_{O2}(\mathrm{k}_{2f} + \mathrm{k}_{3f})\mathrm{x}_A + (\mathrm{k}_{2f}/\mathrm{K}_2)\mathrm{x}_D + (\mathrm{k}_{3f}/\mathrm{K}_3)\mathrm{x}_B - \mathrm{k}_5\mathrm{x}_A^2,$$

$$\dot{\mathrm{x}}_B = \mathrm{k}_{3f}\mathrm{c}_{O2}\mathrm{x}_A - (\mathrm{k}_{3f}/\mathrm{K}_3 + \mathrm{k}_4)\mathrm{x}_B, \qquad \dot{\mathrm{x}}_D = \mathrm{k}_{2f}\mathrm{c}_{O2}\mathrm{x}_A - (\mathrm{k}_{2f}/\mathrm{K}_2)\mathrm{x}_D,$$

$$\dot{\mathrm{x}}_Y = -\mathrm{k}_{1s}\mathrm{x}_Y\mathrm{x}_Z, \qquad \dot{\mathrm{x}}_Z = -\mathrm{k}_1\mathrm{x}_Y\mathrm{x}_Z,$$

*(Decision Variables)* $\mathbf{u} = (\mathrm{k}_{2f}, \mathrm{k}_{3f}, \mathrm{k}_4)$

*(State Variables)* $\mathbf{x} = (\mathrm{x}_A, \mathrm{x}_B, \mathrm{x}_D, \mathrm{x}_Y, \mathrm{x}_Z)$

*(Parameters)* $\mathrm{k}_1, \mathrm{k}_{1s}, \mathrm{k}_5, \mathrm{K}_2, \mathrm{K}_3, \mathrm{c}_{O2}, \Delta\mathrm{t}, \mathrm{n}$

*(Initial Condition)* $\dot{\mathbf{x}}(\mathrm{t} = 0) = (0, 0, 0, 0.4, 140)$


3. Mitsos et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601
6. Wilhelm, ME; Le, AV; and Stuber. MD. "**Global Optimization of Stiff Dynamical Systems.**" *AIChE Journal: Futures Issue,* 65 (12), *2019*
32. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
39. J. W. Taylor, et al. **Direct measurement of the fast, reversible addition of oxygen to cyclohexadienyl radicals in nonpolar solvents**, *Phys. Chem. A*, 108 (2004), pp. 7193–7203.
40. A. B. Singer et al., **Global dynamic optimization for parameter estimation in chemical kinetics** A. B. Singer et al., *J. Phys. Chem. A*, 110 (2006), pp. 971–976

# Kinetic Problem - Formulation

*(Objective Function)*

$$\Phi^* = \min_{\boldsymbol{p} \in P} \sum_{i}^{n} \left(\mathrm{I}^i - \mathrm{I}^i_{data}\right)^2$$

$s.t. \quad \mathrm{I}^i =$

*(Description of Problem)*

- Fit the rate constants ($k_{2f}$, $k_{3f}$, $k_4$) of oxygen addition to cyclohexadienyl radicals to data.[39]

*(pODE IVP)*

$\dot{x}_A = k_1$ …

$\dot{x}_B = k_{3f}$ …

$\dot{x}_Y = -k$ …

… $, k_4)$

… $_D, x_Y, x_Z)$

… $K_3, c_{O2}, \Delta t, n$

… $, 0, 0, 0.4, 140)$

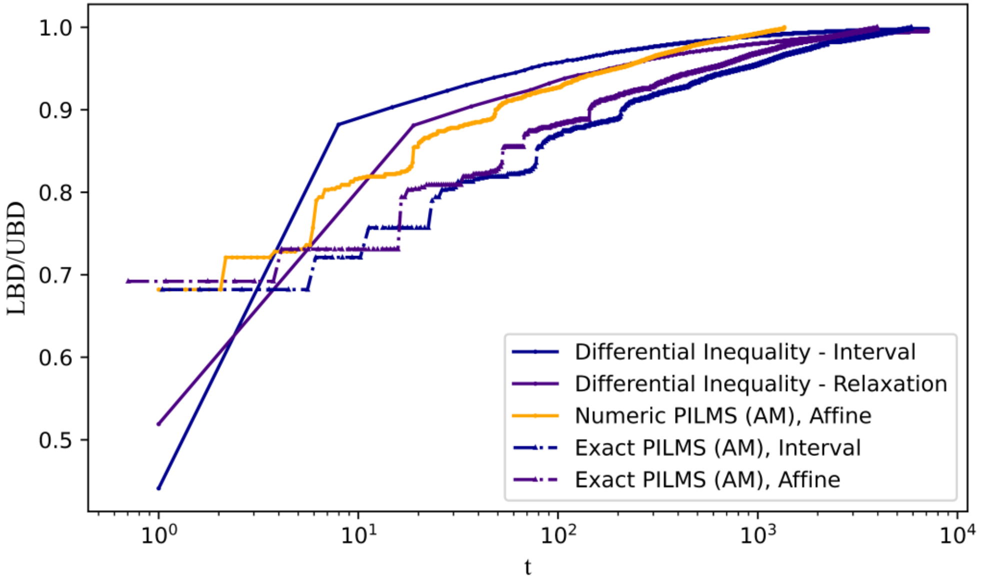
- Affine relaxations used to compute lower bound (CPLEX 12.8).
- Upper-bound computed by integrating ODE at midpoint of active node then evaluating objective & constraints.
- Duality-based bound tightening was performed in all cases.
- Absolute and relative convergence tolerances for the B&B algorithm of $10^{-2}$ and $10^{-5}$, respectively.


3. Mitsos et al. M…
6. Wilhelm, ME; Le, …
32. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
39. J. W. Taylor, et al. **Direct measurement of the fast, reversible addition of oxygen to cyclohexadienyl radicals in nonpolar solvents**, *Phys. Chem. A*, 108 (2004), pp. 7193–7203.
40. A. B. Singer et al., **Global dynamic optimization for parameter estimation in chemical kinetics** A. B. Singer et al., *J. Phys. Chem. A*, 110 (2006), pp. 971–976

# Kinetic Problem - Results

- A comparison of our new approach is made to existing methods.
- The 200 step numerical Adams-Moulton (AM, 2nd order) approach of Wilhelm 2019 is compared to the exact bounds of the solution set with the novel method.
- Differential inequality used approaches using the CVODE Adams integrator (SUNDIALS)[41] are included for comparison.

| Method | Lower Bound | Final Relative Gap | Time (s) | Iterations |
| --- | --- | --- | --- | --- |
| Exact PILMS, Adams-Moulton | Interval | None | 5983 | >800,000 |
| Exact PILMS, Adams-Moulton | Affine | None | 3976 | >350,000 |
| Numerical, Adams-Moulton, 200 step | Affine | None | 1356 | 6068 |
| Differential Inequality | Interval[6,7,9] | 1.9E-3 | >7200 | >1,300,000 |

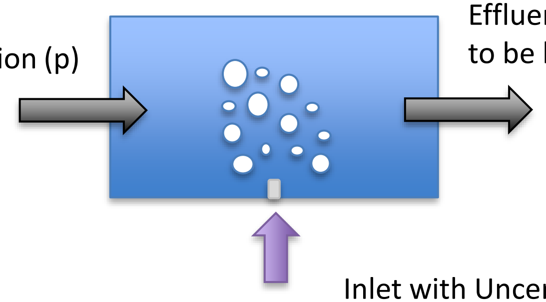




41. Serban, Radu, and Alan C. Hindmarsh. **CVODES: the sensitivity-enabled ODE solver in SUNDIALS.** *International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*. Vol. 47438. 2005.
32. Wilhelm, ME; Le, AV; and Stuber. MD. "**Global Optimization of Stiff Dynamical Systems.**" *AIChE Journal: Futures Issue,* 65 (12), *2019*
9. Harrison, Gary W. **Dynamic models with uncertain parameters.** *Proceedings of the first international conference on mathematical modeling.* Vol. 1. University of Missouri Rolla, 1977.
10. W. Walter. **Differential and integral inequalities** *Springer-Verlag*, New York (1970)
11. Scott, Joseph K., and Paul I. Barton. **Bounds on the reachable sets of nonlinear control systems.** *Automatica* 49.1 (2013): 93-100.
12. Scott, Joseph K., and Paul I. Barton. **Improved relaxations for the parametric solutions of ODEs using differential inequalities.** *Journal of Global Optimization* 57.1 (2013): 143-176.

# Robust Design - SIP

### *CSTR with Aeration*




### *Goal*

Minimize aeration cost while ensuring constraint satisfaction at final time ($t = 500\ s$) if step-change feed disturbance occurs

$$\Phi^* = \min_{u \in U} u$$
$$s.t.\ x_1(t_f, u, p) - SP \leq 0, \forall p \in P$$

### *Initial Condition*

Steady-state operation with $x_1$ = 30 (mg/L)

### *Mass balance*

$$\frac{dx_1}{dt} = \tau^{-1}(p - x_1) - r_{AO}X_{AO}$$
$$\frac{dx_2}{dt} = r_{AO}X_{AO} - r_{NO}(x_2, x_4)X_{NO}$$
$$\frac{dx_3}{dt} = r_{NO}(x_2, x_4)X_{NO}$$
$$\frac{dx_4}{dt} = -r_{AO}\Psi_{AO}X_{AO} - r_{NO}(x_2, x_4)\Psi_{NO}X_{NO} + ku(C_O^* - x_4)$$

### *Rate Law*

$$r_{NO} = r_{NO,max}\frac{x_2}{K_{SNO} + x_2 + {x_2}^2/K_{INO}}\frac{x_4}{K_{ONO} + x_4}$$

### *Variable Range*

$$P = [31,40], \qquad U = [440,2000], \qquad t = [0,500]$$

42. Matthew E. Wilhelm, Chenyu Wang, and Matthew D. Stuber. **Robust Optimization with Hybrid First-Principles Data-Driven Models.** *Computers and Chemical Engineering. Under review.*

# Comparison of Methods

- Optimal aeration rate found to be $u = 704\ L/s$ via algorithms compared.
- Exact PILMs methods faster than numerical approximation.
- Exact PILMs comparable to differential inequality method.

| Method | Lower Bound | Time (s) |
|---|---|---|
| Exact PILMS, Adams-Moulton | Interval | 55 |
| Exact PILMS, Adams-Moulton | Affine | 36 |
| Numerical, Adams-Moulton, 200 step | Interval | 323 |
| Numerical, Adams-Moulton, 200 step | Affine | 118 |
| Differential Inequality | Interval | 38 |

| Parameter | Value | Reference |
|---|---|---|
| Residence time (τ) | 4136 | - |
| Saturated Oxygen Concentration ($C_O^*$) | 9.1 | Rodger B. Baird, Andrew D. Eaton, and Eugene W. Rice. **Standard Methods for the Examination of Water and Wastewater.** *APHA, AWWA, and WEF,* Washington, D.C., 2017. |
| Concentration of AOB ($X_{AO}$) | 505 | Omar Sánchez, et al**. The effect of sodium chloride on the two-step kinetics of the nitrifying process.** *Water Environment Research*, 76(1):73–80. |
| Concentration of NOB ($X_{NO}$) | 151 | |
| Maximum Nitrite Consumption Rate ($r_{NO,max}$) | 1.07 | |
| Stoichiometric ratio $O_2$:$NH_4$ ($\Psi_{AO}$) | 2.5 | Udo Wiesmann. **Biological nitrogen removal from wastewater.** *In Biotechnics / Wastewater,* pages 113–154. Springer Berlin Heidelberg, 1994. |
| Stoichiometric ratio $O_2$:$NO_2^-$ ($\Psi_{NO}$) | 0.32 | |
| Monod constant of $NO_2$ for NOB ($K_{SNO}$) | 1.6 | |
| Inhibition constant of $NO_2$ for NOB ($K_{INO}$) | 13000 | |
| Monod constant of $O_2$ for NOB ($K_{ONO}$) | 1.5 | |
| Lumped aeration constant (k) | 3.26E-6 | Lars Uby. **Next steps in clean water oxygen transfer testing – a critical review of current standards.** *Water Research*,157:415–434, 2019. |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