Carnegie Mellon University

CAPD CENTER

Decomposition method for the Multiperiod Blending Problem

Irene Lotero, Francisco Trespalacios and Ignacio Grossmann

September 17-18, 2014

Center for Advanced Process Decision-making
Department of Chemical Engineering Carnegie Mellon University
Pittsburgh, PA 15213

Outline

Background

- Problem description
- Applications
- Mathematical Formulation

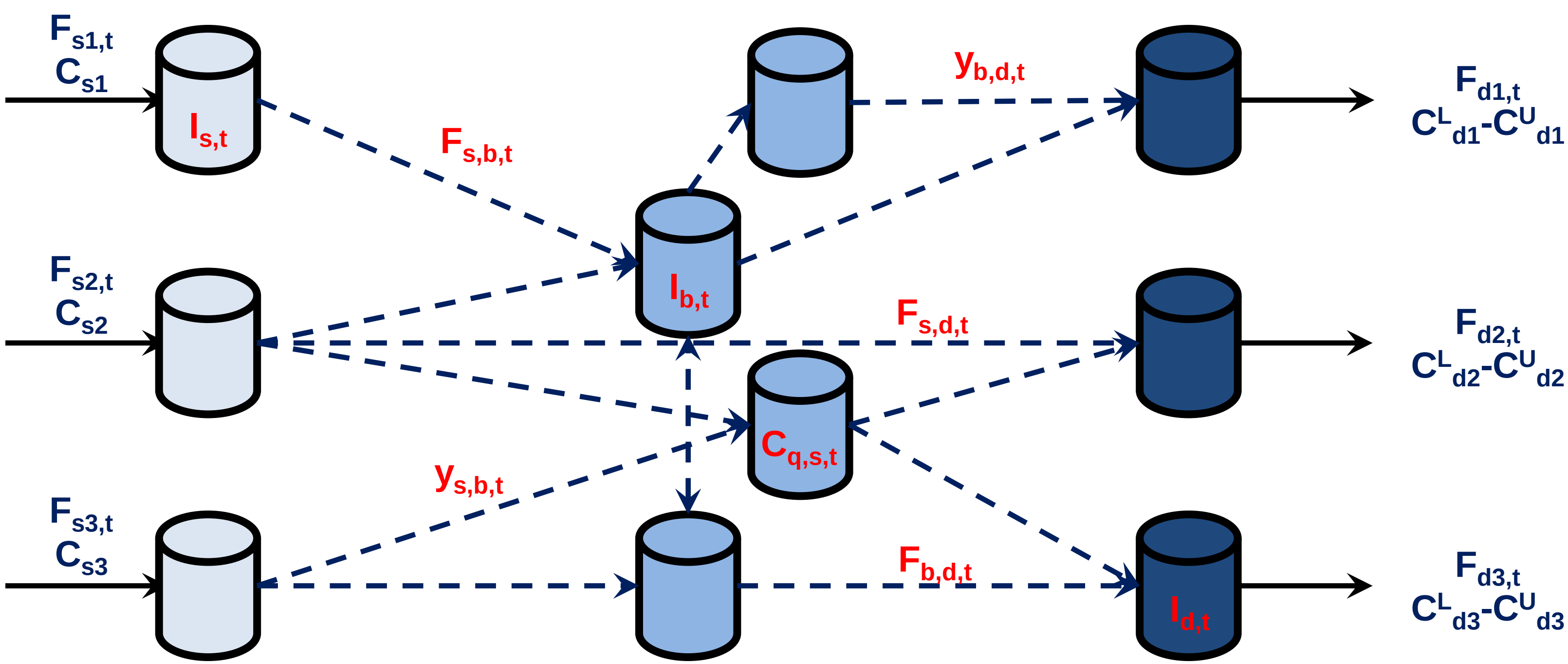
Motivation

- State-of-the-art commercial MINLP solvers struggle
- Generate “good” solutions fast

Approach

- Alternative mathematical formulation based on GDP
- Decomposition algorithm

Multiperiod blending problem is defined over supply, blending and demand tanks

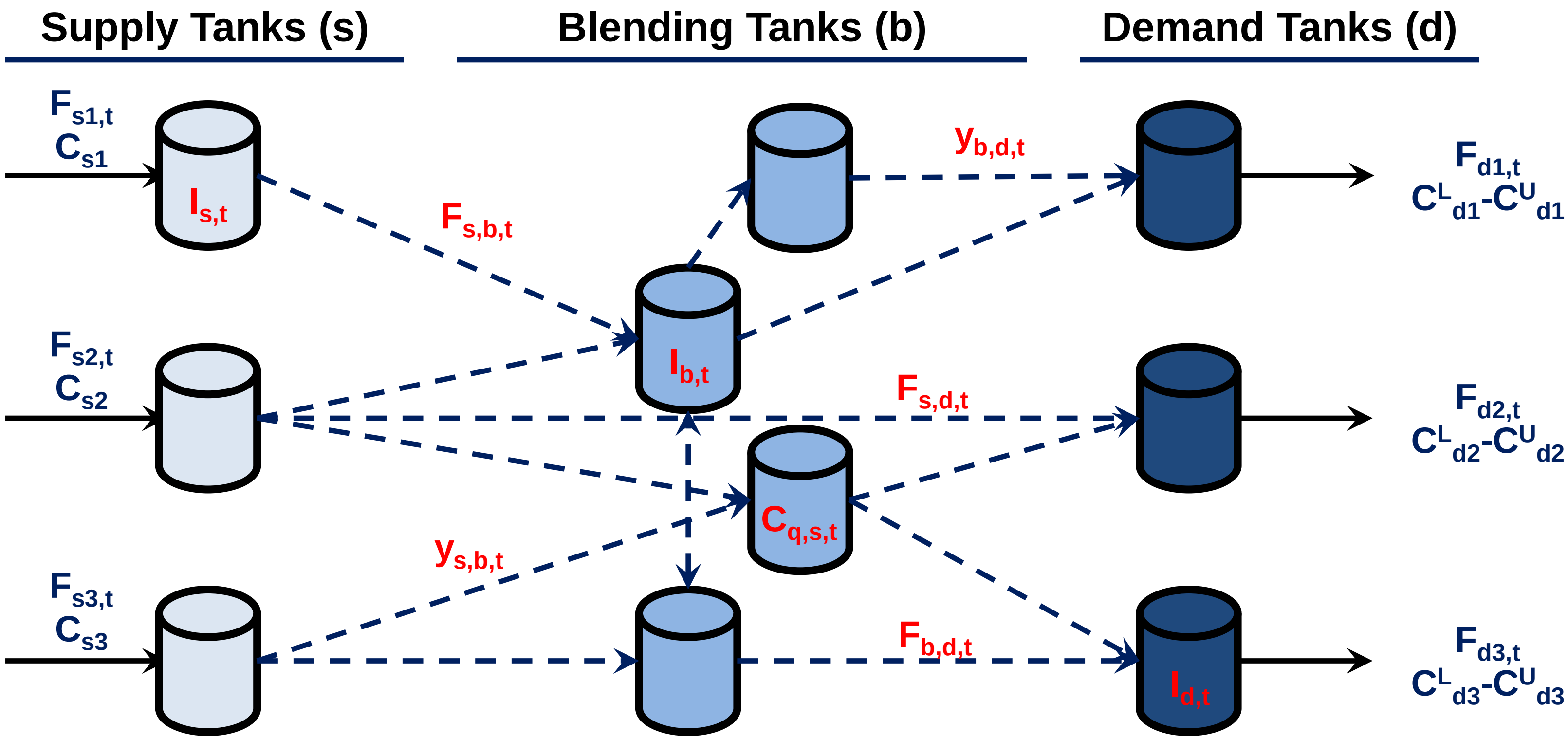


Given:
- Topology, initial conditions and flow profit/costs
- Supply tank flow and concentration
- Demand tank flow and concentration limits

Determine
- Flows between which tanks in which time periods
- Inventories/concentrations for tanks in each period
- **Maximum total profit of blending operation**

Assumptions:
- Supply concentrations are constant
- Perfect mixing
- **No simultaneous input/output to blending tanks**

General model for many applications



Applications

- Gasoline and crude oil blending
- Raw material feed scheduling
- Storage of intermediate streams
- Water treatment
- Emissions regulation

Nomenclature

$I_{n,t}$	Inventory for tank n at time t
$F_{nn't}$	Flow between tanks n and n' at time t
C_{qnt}	Concentration of quality q of tank n at time t
$y_{nn't}$	Flow indicator between tank n and n' at time

MINLP formulation contains bilinear terms

Type

max profit - network flow cots

$$\max \sum_{t\in T}\left[\sum_{n\in S\cup B}\sum_{d\in D}\beta_d F_{ndt} - \sum_{s\in S}\sum_{n\in B\cup D}\beta_s F_{snt} - \sum_{nn'\in N}(\alpha_{nn'}y_{nn't}+\beta_{nn'}F_{nn't})\right]$$

Type: linear

s.t

for flows into blending tanks:

[flow within bounds] ∨ [flow = 0]

$$\begin{bmatrix} Y_{nn't} \\ F^L_{nn'} \le F_{nn't} \le F^U_{nn'} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{nn't} \\ F_{nn't} = 0 \end{bmatrix} \qquad \forall\, nn'\epsilon(BB\cup SB), t\epsilon T$$

Type: mixed-integer linear

for flows into demand tanks:

[flow within bounds, concentrations within demand spec.] ∨ [flow = 0, "no bounds" on concentration]

$$\begin{bmatrix} Y_{bdt} \\ C^L_{qd} \le C_{qbt-1} \le C^U_{qd} \\ F^L_{bd} \le F_{bdt} \le F^U_{bd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{bdt} \\ 0 \le C_{qbt-1} \le 1 \\ F_{bdt} = 0 \end{bmatrix} \qquad \forall\, b\epsilon B, d\epsilon D, q\epsilon Q, t\epsilon T$$

$$\begin{bmatrix} Y_{sdt} \\ C^L_{qd} \le C^{IN}_{qs} \le C^U_{qd} \\ F^L_{sd} \le F_{sdt} \le F^U_{sd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{sdt} \\ 0 \le C^{IN}_{qs} \le 1 \\ F_{sdt} = 0 \end{bmatrix} \qquad \forall\, s\epsilon S, d\epsilon D, q\epsilon Q, t\epsilon T$$

Type: mixed-integer linear

total inventory mass balance in tanks

$$I_{st} = I_{st-1} + F^{IN}_{st} - \textstyle\sum_{n\epsilon B\cup D} F_{snt} \qquad \forall\, s\epsilon S, t\epsilon T$$

$$I_{bt} = I_{bt-1} + \textstyle\sum_{n\epsilon S\cup B} F_{nbt} - \sum_{n\epsilon B\cup D} F_{bnt} \qquad \forall\, b\epsilon B, t\epsilon T$$

$$I_{dt} = I_{dt-1} + \textstyle\sum_{n\epsilon S\cup B} F_{ndt} - F^{OUT}_{dt} \qquad \forall\, d\epsilon D, t\epsilon T$$

Type: linear

Contains bilinear terms, for each contaminant, each blending tank and each time period

inventory mass balance by component in blending tanks

$$I_{bt}C_{qbt} = I_{bt-1}C_{qbt-1} + \sum_{s\epsilon S} F_{sbt}C^{IN}_{qs} + \sum_{b'\epsilon B} F_{b'bt}C_{qb't-1} - \sum_{n\epsilon B\cup D} F_{bnt}C_{qbt-1}$$

Type: nonlinear (nonconvex)

no simultaneous in/out flow

$$Y_{nbt} \Rightarrow \neg Y_{bn't} \qquad \forall\, b\epsilon B, n\epsilon S\cup B, n'\epsilon B\cup D, t\epsilon T$$

Type: integer linear

variable bounds

$$0 \le I_{nt} \le I^U_n;\ 0 \le F_{nn't};\ 0 \le C_{qbt} \le 1 \qquad \forall\, n\epsilon TA, t\epsilon T$$

$$Y_{nn't}\,\epsilon\{True, False\} \qquad \forall\, nn'\epsilon N, t\epsilon T$$

Type: linear

Outline

Background

- Problem description
- Applications
- Mathematical Formulation

Motivation

- State-of-the-art commercial MINLP solvers struggle
- Generate “good” solutions fast

Approach

- Alternative mathematical formulation based on GDP
- Decomposition algorithm

Commercial solvers not able to find feasible solutions

Commercial Solvers Performance

- **36 randomly generated instances**
- **After 5 minutes** of computational time,

	Average normalized best feasible solution
Optimal	1.0
GloMIQO	0.57
BARON	0.19
SCIP	0.35

- **After 30 minutes** of computational time,

	Found Feasible Solution Large Instances
GloMIQO	54%
BARON	0%
SCIP	15%

Objectives

Increase size of the problems

- **Current problems**: 4 time periods
  8 qualities
  4 blending tanks
- **Target problems:** 12 time periods
  10 qualities
  16 blending tanks

Generate "good solutions" fast

- Guaranteeing global optimality not a priority
- Obtain good feasible solutions

Outline

Background

- Problem description
- Applications
- Mathematical Formulation

Motivation

- State-of-the-art commercial MINLP solvers struggle
- Generate “good” solutions fast

Approach

- Alternative mathematical formulation based on GDP
- Decomposition algorithm

GDP is a higher level of representation for MILP/MINLP

Optimization problem with algebraic expressions, disjunctions & logic propositions

General form of GDP[1]

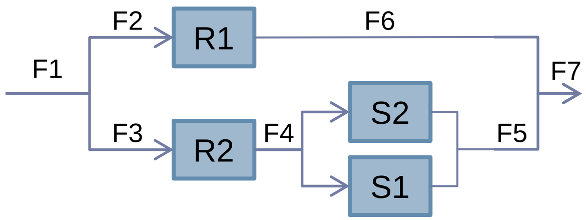
$$\min z = f(x)$$ *Objective Function*

$$s.t.\ g(x) \leq 0$$ *Global Constraints*

$$\vee_{i \in D_k} \begin{bmatrix} Y_{ki} \\ r_{ki}(x) \leq 0 \end{bmatrix} \quad k \in K$$ *Disjunctions*

$$\Omega(Y) = True$$ *Logic Propositions*

Illustration – Process network



$$\max z = P_7F_7 - P_1F_1 - c_R - c_S$$ *Objective function*

$$F_1 = F_2 + F_3$$
$$F_7 = F_5 + F_6$$ *Global Constraints*

$$\begin{bmatrix} Y_{R1} \\ F_6 = \beta_{R1}F_2 \\ F_3 = F_4 = 0 \\ c_R = \gamma_{r1} \end{bmatrix} \vee \begin{bmatrix} Y_{R2} \\ F_6 = F_2 = 0 \\ F_4 = \beta_{R2}F_3 \\ c_R = \gamma_{r2} \end{bmatrix}$$

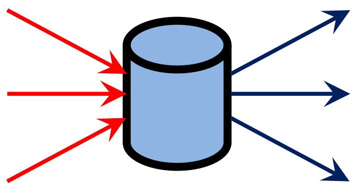
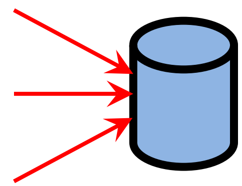
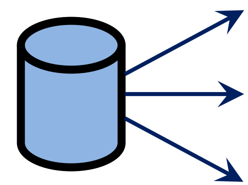
$$\begin{bmatrix} Y_{S1} \\ F_5 = \beta_{S1}F_4 \\ c_S = \gamma_{s2} \end{bmatrix} \vee \begin{bmatrix} Y_{S2} \\ F_5 = \beta_{S2}F_4 \\ c_S = \gamma_{s2} \end{bmatrix} \vee \begin{bmatrix} Y_{S\_NO} \\ F_5 = 0 \\ c_S = 0 \end{bmatrix}$$ *Disjunctions*

$$Y_{R1} \Leftrightarrow Y_{S\_NO}$$ *Logic*

1. Raman R. and Grossmann I.E., "Modelling and Computational Techniques for Logic-Based Integer Programming", Computers and Chemical Engineering, 18, 563, 1994.

Remark: Possible to reduce bilinear terms using a disjunction

Requires 0-1 variable, but it does not increase combinatorial complexity (it might even reduce it!)[1]

	Blend + Split tank		Blending tank		Split tank
Tank				V	
Mass balance	$I_{bt} = I_{bt-1} + \sum_{n \epsilon SUB} F_{nbt} - \sum_{n \epsilon BUD} F_{bnt}$		$I_{bt} = I_{bt-1} + \sum_{n \epsilon SUB} F_{nbt}$		$I_{bt} = I_{bt-1} - \sum_{n \epsilon BUD} F_{bnt}$
Comp. mass balance	$I_{bt} C_{qbt} = I_{bt-1} C_{qbt-1} + \sum_{s \epsilon S} F_{sbt}\, C_{qs}^{IN} + \sum_{b' \epsilon B} F_{b'bt} C_{qb't-1} - \sum_{n \epsilon BUD} F_{bnt} C_{qbt-1}$		$I_{bt} C_{qbt} = I_{bt-1} C_{qbt-1} + \sum_{s \epsilon S} F_{sbt}\, C_{qs}^{IN} + \sum_{b' \epsilon B} F_{b'bt} C_{qb't-1}$		$C_{qbt} = C_{qbt-1}$ Fewer or none bilinear terms

If some of the tanks are fixed as "split tanks", the resulting MINLP becomes easier to solve

1. The new binary variable can in fact be continuous due to the problem structure. Furthermore, using it as binary variable and giving it priority over the network variables can increase the solution time of a branch-and-bound method

Original MINLP formulation

Type

$$Max \sum_{t\epsilon T}\left[\sum_{n\epsilon SUB}\sum_{d\epsilon D}\beta_d F_{ndt} - \sum_{s\epsilon S}\sum_{n\epsilon B\cup D}\beta_s F_{snt} - \sum_{nn'\epsilon N}(\alpha_{nn'}y_{nn't} + \beta_{nn'}F_{nn't})\right]$$

linear

s.t

$$\begin{bmatrix} Y_{nn't} \\ F^L_{nn'} \le F_{nn't} \le F^U_{nn'} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{nn't} \\ F_{nn't} = 0 \end{bmatrix} \qquad \forall\, nn'\epsilon(BB \cup SB), t\epsilon T$$

mixed-integer linear

$$\begin{bmatrix} Y_{bdt} \\ C^L_{qd} \le C_{qbt-1} \le C^U_{qd} \\ F^L_{bd} \le F_{bdt} \le F^U_{bd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{bdt} \\ 0 \le C_{qbt-1} \le 1 \\ F_{bdt} = 0 \end{bmatrix} \qquad \forall\, b\epsilon B, d\epsilon D, q\epsilon Q, t\epsilon T$$

$$\begin{bmatrix} Y_{sdt} \\ C^L_{qd} \le C^{IN}_{qs} \le C^U_{qd} \\ F^L_{sd} \le F_{sdt} \le F^U_{sd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{sdt} \\ 0 \le C^{IN}_{qs} \le 1 \\ F_{sdt} = 0 \end{bmatrix} \qquad \forall\, s\epsilon S, d\epsilon D, q\epsilon Q, t\epsilon T$$

mixed-integer linear

$$I_{st} = I_{st-1} + F^{IN}_{st} - \sum\nolimits_{n\epsilon B\cup D} F_{snt} \qquad \forall\, s\epsilon S, t\epsilon T$$

$$I_{bt} = I_{bt-1} + \sum\nolimits_{n\epsilon S\cup B} F_{nbt} - \sum\nolimits_{n\epsilon B\cup D} F_{bnt} \qquad \forall\, b\epsilon B, t\epsilon T$$

$$I_{dt} = I_{dt-1} + \sum\nolimits_{n\epsilon S\cup B} F_{ndt} - F^{OUT}_{dt} \qquad \forall\, d\epsilon D, t\epsilon T$$

linear

$$I_{bt}C_{qbt} = I_{bt-1}C_{qbt-1} + \sum_{s\epsilon S} F_{sbt}C^{IN}_{qs} + \sum_{b'\epsilon B} F_{b'bt}C_{qb't-1} - \sum_{n\epsilon B\cup D} F_{bnt}C_{qbt-1}$$

nonlinear (nonconvex)

$$Y_{nbt} \Rightarrow \neg Y_{bn't} \qquad \forall\, b\epsilon B, n\epsilon S \cup B, n'\epsilon B \cup D, t\epsilon T$$

integer linear

$$0 \le I_{nt} \le I^U_n \quad 0 \le F_{nn't}; 0 \le C_{qbt} \le 1 \qquad \forall\, n\epsilon TA, t\epsilon T$$

$$Y_{nn't}\epsilon\{True, False\} \qquad \forall\, nn'\epsilon N, t\epsilon T$$

linear

Alternative MINLP formulation based on GDP

Type

$$Max \sum_{t\epsilon T}\left[\sum_{n\epsilon S\cup B}\sum_{d\epsilon D}\beta_d F_{ndt} - \sum_{s\epsilon S}\sum_{n\epsilon B\cup D}\beta_s F_{snt} - \sum_{nn'\epsilon N}(\alpha_{nn'}y_{nn't} + \beta_{nn'}F_{nn't})\right]$$ linear

s.t

$$\begin{bmatrix} Y_{nn't} \\ F^L_{nn'} \le F_{nn't} \le F^U_{nn'} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{nn't} \\ F_{nn't} = 0 \end{bmatrix} \quad \forall\, nn'\epsilon(BB \cup SB), t\epsilon T$$ mixed-integer linear

$$\begin{bmatrix} Y_{bdt} \\ C^L_{qd} \le C_{qbt-1} \le C^U_{qd} \\ F^L_{bd} \le F_{bdt} \le F^U_{bd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{bdt} \\ 0 \le C_{qbt-1} \le 1 \\ F_{bdt} = 0 \end{bmatrix} \quad \forall\, b\epsilon B, d\epsilon D, q\epsilon Q, t\epsilon T$$

$$\begin{bmatrix} Y_{sdt} \\ C^L_{qd} \le C^{IN}_{qs} \le C^U_{qd} \\ F^L_{sd} \le F_{sdt} \le F^U_{sd} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{sdt} \\ 0 \le C^{IN}_{qs} \le 1 \\ F_{sdt} = 0 \end{bmatrix} \quad \forall\, s\epsilon S, d\epsilon D, q\epsilon Q, t\epsilon T$$ mixed-integer linear

$$I_{st} = I_{st-1} + F^{IN}_{st} - \textstyle\sum_{n\epsilon B\cup D} F_{snt} \quad \forall\, s\epsilon S, t\epsilon T$$

$$I_{dt} = I_{dt-1} + \textstyle\sum_{n\epsilon S\cup B} F_{ndt} - F^{OUT}_{dt} \quad \forall\, d\epsilon D, t\epsilon T$$ linear

Implies decomposition

$$\begin{bmatrix} YB_{bt} \\ I_{bt} = I_{bt-1} + \sum_{n\epsilon S\cup B} F_{nbt} \\ I_{bt}C_{qbt} = I_{bt-1}C_{qbt-1} + \sum_{s\epsilon S} F_{sbt}\, C^{IN}_{qs} + \sum_{b'\epsilon B} F_{b'bt}C_{qb't-1} \\ \forall\, q\epsilon Q \end{bmatrix} \vee \begin{bmatrix} \neg YB_{bt} \\ I_{bt} = I_{bt-1} - \sum_{n\epsilon B\cup D} F_{bnt} \\ C_{qbt} = C_{qbt-1} \quad \forall\, q\epsilon Q \end{bmatrix}$$ nonlinear (nonconvex)

$$Y_{nbt} \Rightarrow YB_{bt} \quad \forall\, b\epsilon B, n\epsilon S \cup B, t\epsilon T$$

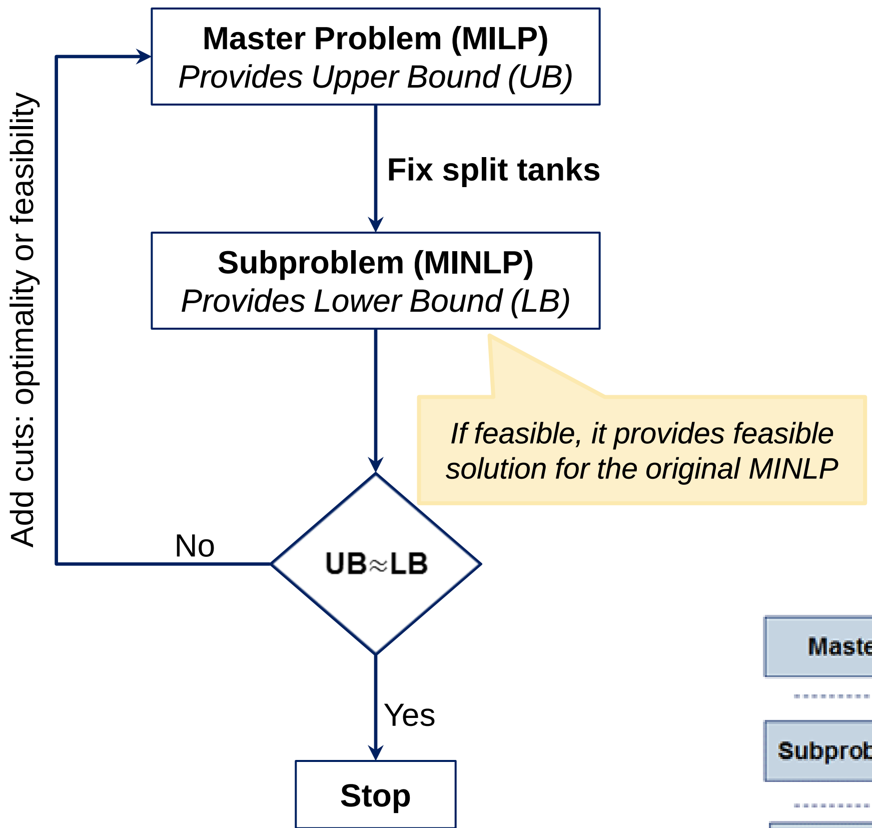
$$Y_{bnt} \Rightarrow \neg YB_{bt} \quad \forall\, b\epsilon B, n\epsilon B \cup D, t\epsilon T$$ integer linear

$$0 \le I_{nt} \le I^U_n \quad 0 \le F_{nn't};\ 0 \le C_{qbt} \le 1 \quad \forall\, n\epsilon TA, t\epsilon T$$ linear

$$Y_{nn't}\epsilon\{True, False\} \quad \forall\, nn'\epsilon N, t\epsilon T$$

Decomposition algorithm seeks to find feasible solutions in short periods of time

Algorithm



Decisions in the algorithm

Master MILP (MINLP relaxation)

- Multiparametric disaggregation[1]

Solving MINLP

- Smaller nonconvex MINLP
- Global solution through specialized technique, e.g. multiparametric disaggregation

Other considerations

- “no-good” are included in the subproblem, eliminating regions already evaluated in previous subproblems

	1st Iteration	2nd Iteration
Master	$\neg YB_1 \wedge \neg YB_3$	$\neg YB_1 \wedge \neg YB_2$
Subproblem	$\neg YB_1 \wedge \neg YB_2 \wedge \neg YB_3$	~~$\neg YB_1 \wedge \neg YB_2 \wedge \neg YB_3$~~
Cut	$Z \leq (1 + YB_1 + YB_3) * LB$	$YB_1 + YB_2 \geq 1$

[2] Kolodziej, S.P., Castro, P.M., Grossmann, I.E. Global optimization of bilinear programs with a multiparametric disaggregation technique. Journal of Global Optimization (2013)

Multiparametric disaggregation provides a lower bound

Discretization Technique

$$w = u * v$$

One of the two terms is discretized (in this case v)

Precision

$$v = 10^{\pi} * \sum_{l=0}^{P} 2^l * z_l$$

Binary variables

$$w = 10^{\pi} * \sum_{l=0}^{P} 2^l * \hat{u}_l$$

$$\left[\hat{u}_l \overset{z_l}{=} u\right] \vee \left[\hat{u}_l \overset{\neg z_l}{=} 0\right]$$

$$u^L * z_l \leq \hat{u}_l \leq u^U * z_l$$
$$u - M(1 - z_l) \leq \hat{u}_l \leq u$$

If approx. MILP is feasible, provides solution for original MINLP

Notes and examples

Example: 0.56 can be represented as:

$(2^5 + 2^4 + 2^3) \cdot 10^{-2} = 0.56$

$z_3 = z_4 = z_5 = 1$. Other $z_l = 0$

$\pi = -2$ and $P = 6$

We can use other bases for more/fewer binary variables

- Base two takes fewer binary variables

Range	0 – 15 0 – 9	0 – 12.7 0 – 9.9	0 – 10.23 0 – 9.99
Increment	1	0.1	0.01
Binary Variables			
Base 2	8	14	20
Base 10	10	20	30

Multiperiod blending problem

Bilnear terms are $F * C$ and $I * C$

Need to select between two options:

- Discretize flow and inventory
- Discretize concentration

Scales up better

Slack variables are introduced for upper bound

Discretization Technique + Slack

$$w = u * v$$

$0 \leq \bar{z} \leq 1$

$$v = 10^{\pi} * \sum_{l=0}^{P} 2^{l} * z_l + 10^{\pi} * \bar{z}$$

$$w = 10^{\pi} * \sum_{l=0}^{P} 2^{l} * \hat{u}_l + 10^{\pi} * \bar{u}$$

$$\begin{bmatrix} z_l \\ \hat{u}_l = u \end{bmatrix} \vee \begin{bmatrix} \neg z_l \\ \hat{u}_l = 0 \end{bmatrix}$$

$$u^L * \bar{z} \leq \bar{u} \leq u^U * \bar{z}$$

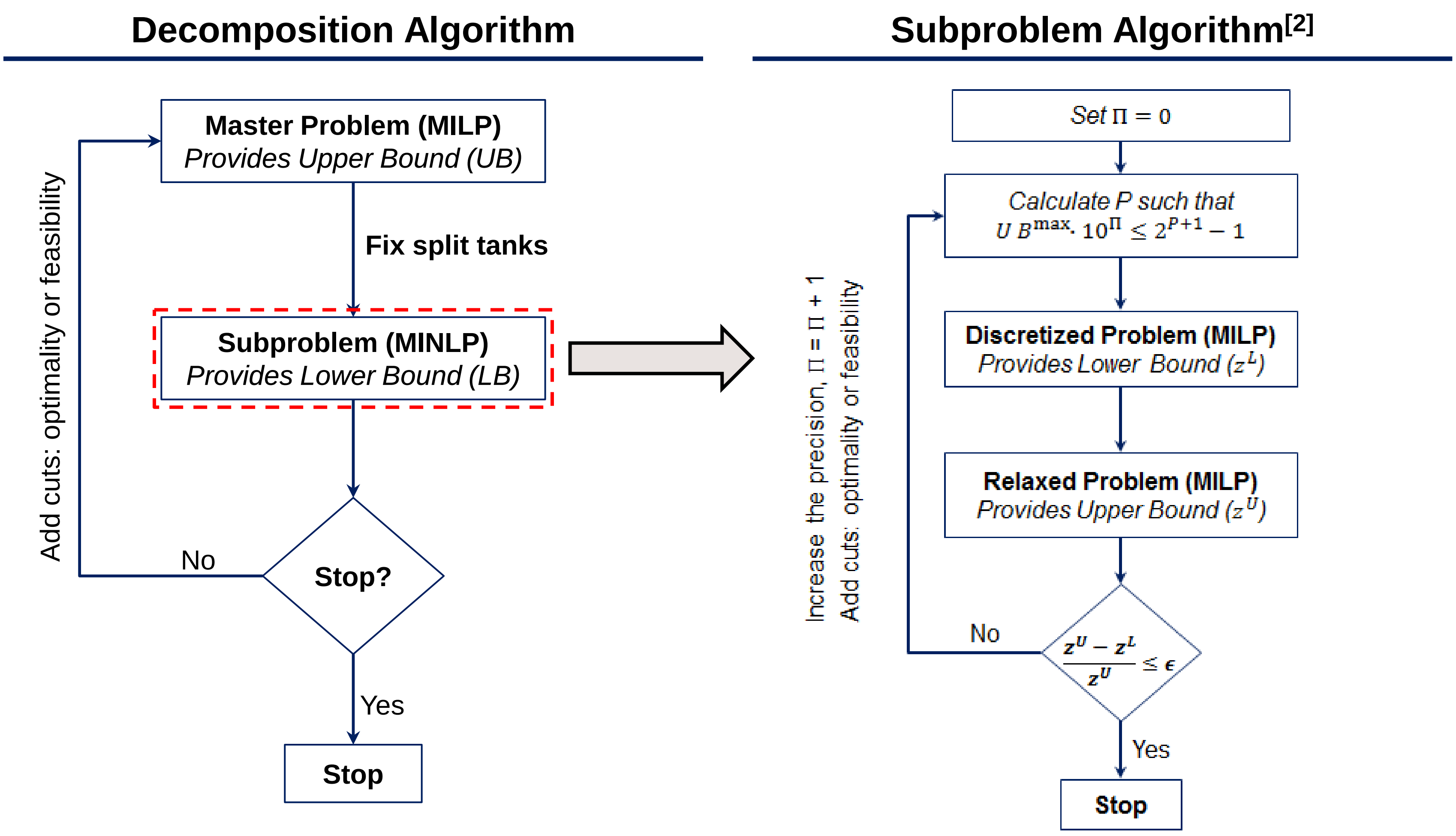
$$u - u^U(1 - \bar{z}) \leq \bar{u} \leq u - u^L(1 - \bar{z})$$

Notes

Is a relaxation problem because it includes at least the entire feasible region of the problem

The relaxed MILP provides a valid upper bound for original MINLP

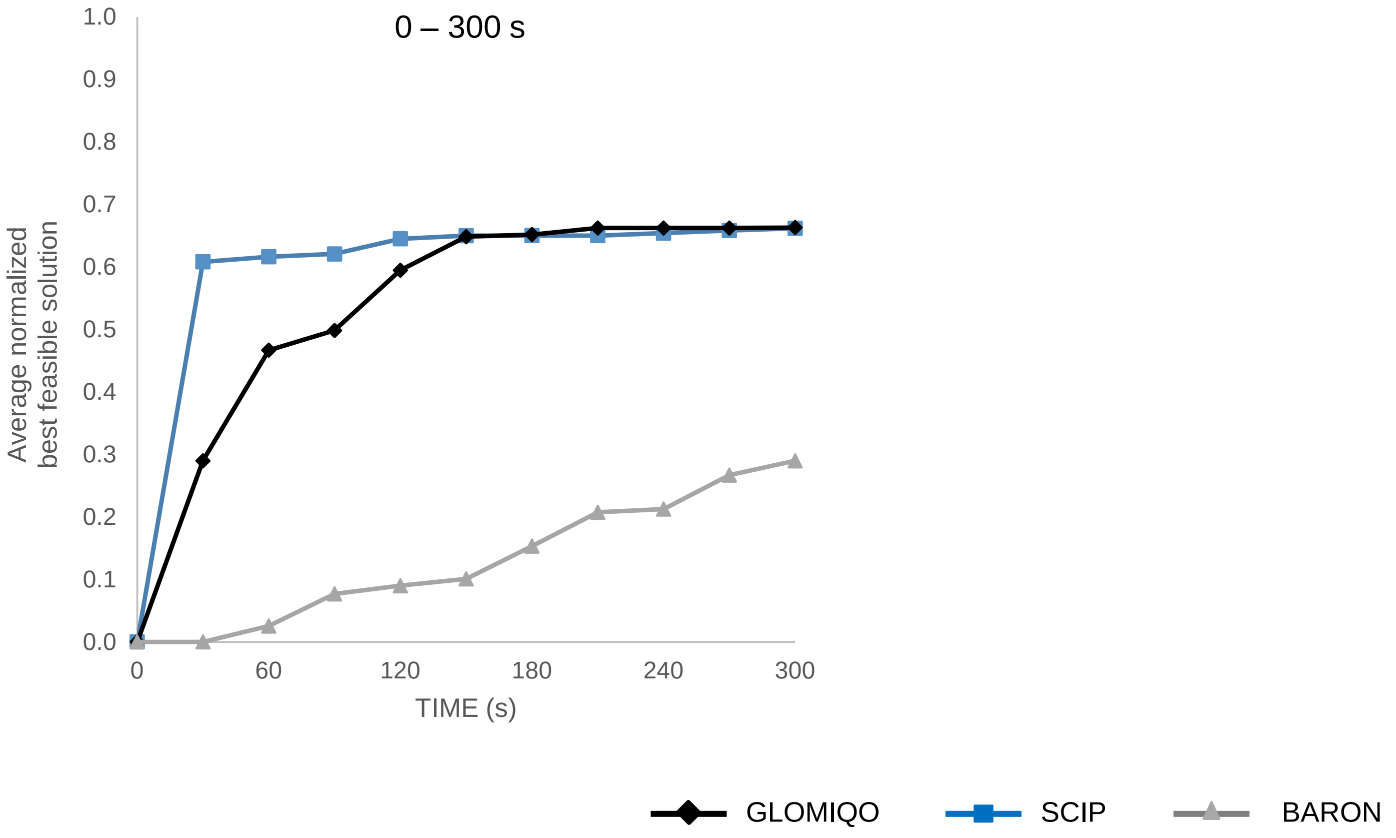
Subproblem algorithm solves the discretized and relaxed MILPs successively increasing the precision



[2] Kolodziej, S.P., Grossmann, I.E., Furman, K.C. and Sawaya, N.W. A discretization-based approach for the optimization of the multiperiod blend scheduling problem, Computers & Chemical Engineering, (2013).

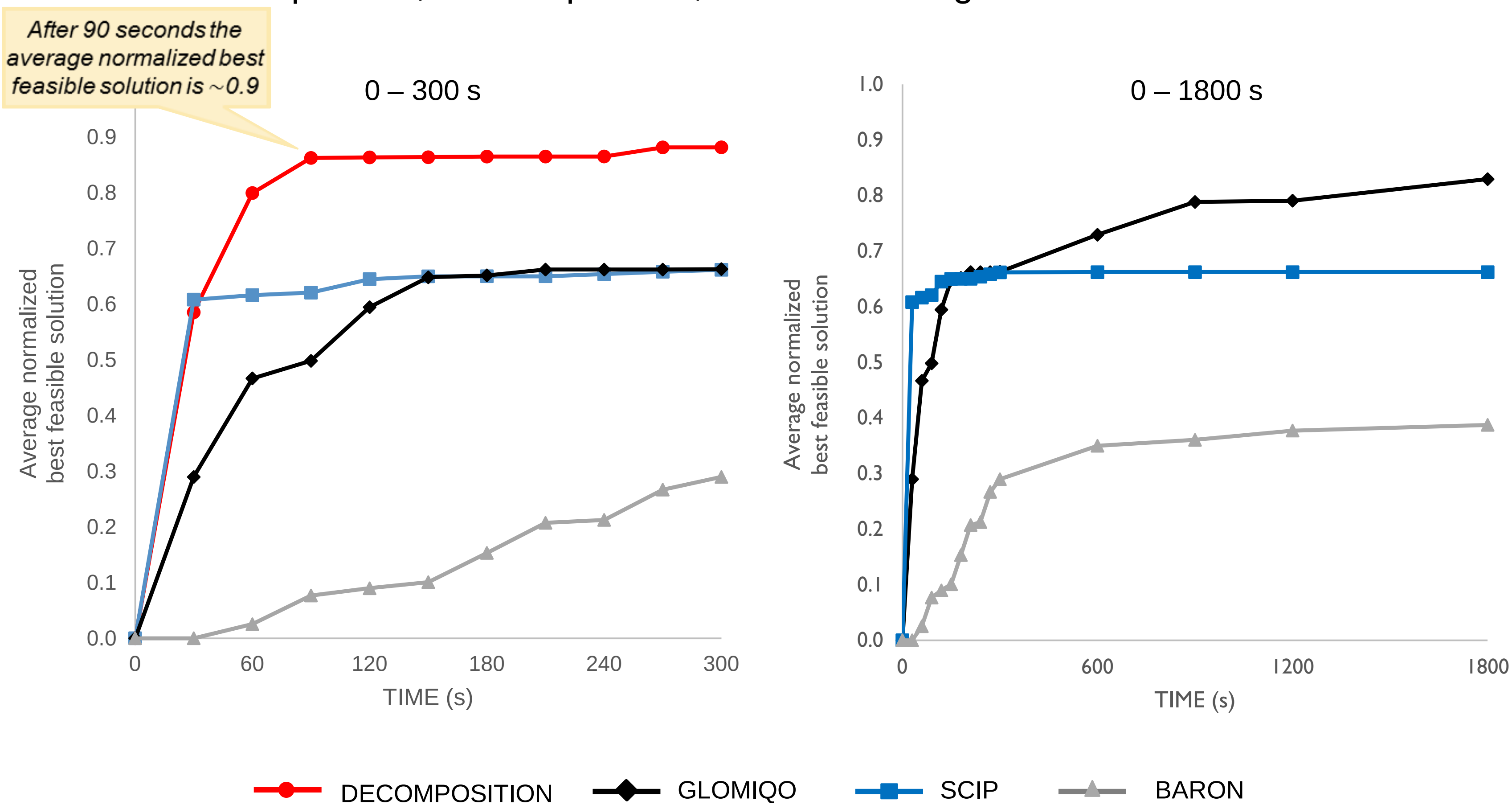
Results Small Instances

- 18 randomly generated instances
- 3 – 4 time periods, 2 – 10 qualities, 4 – 12 blending tanks



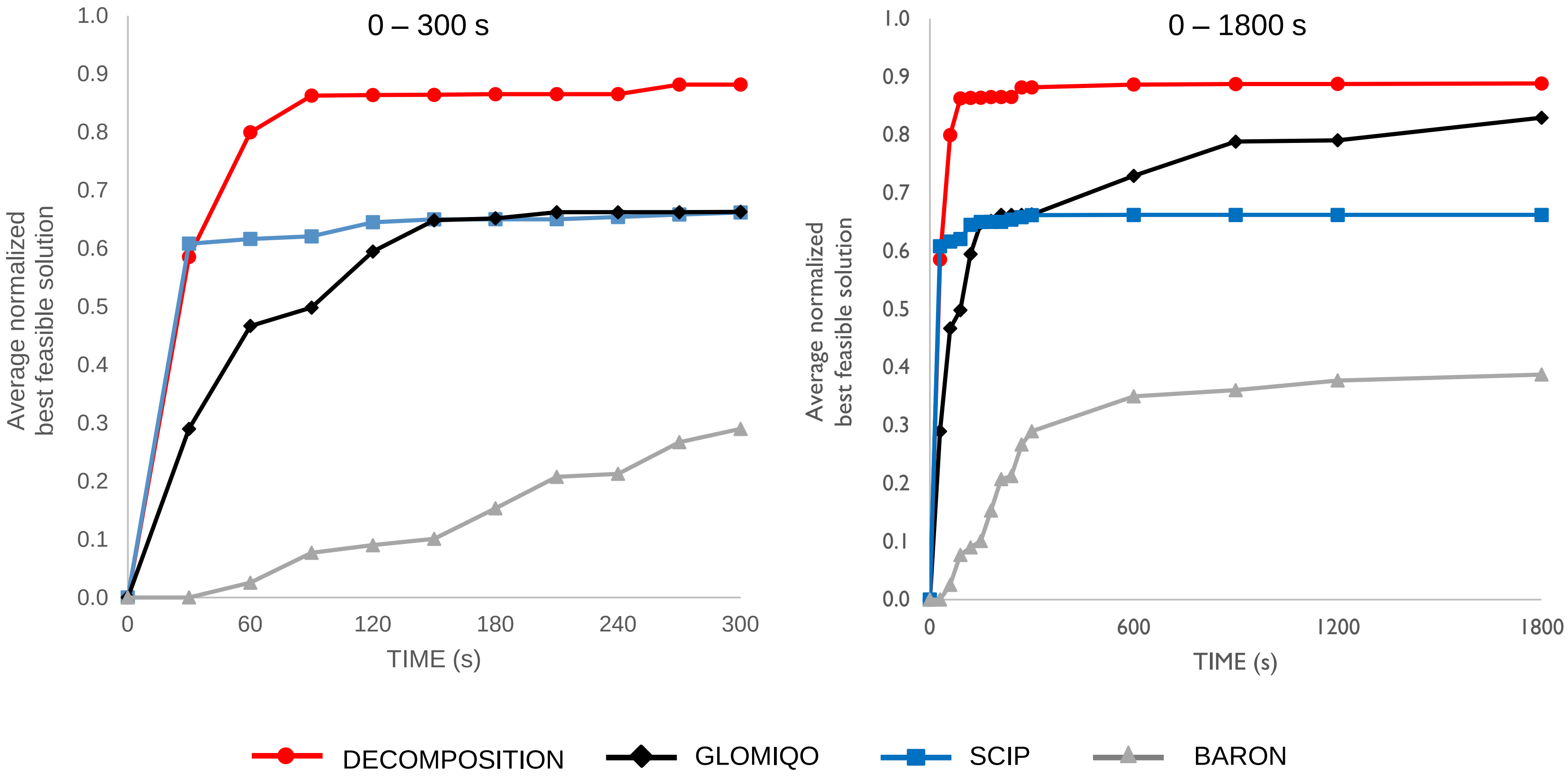
Results Small Instances

- 18 randomly generated instances
- 3 – 4 time periods, 2 – 10 qualities, 4 – 12 blending tanks



Results Small Instances

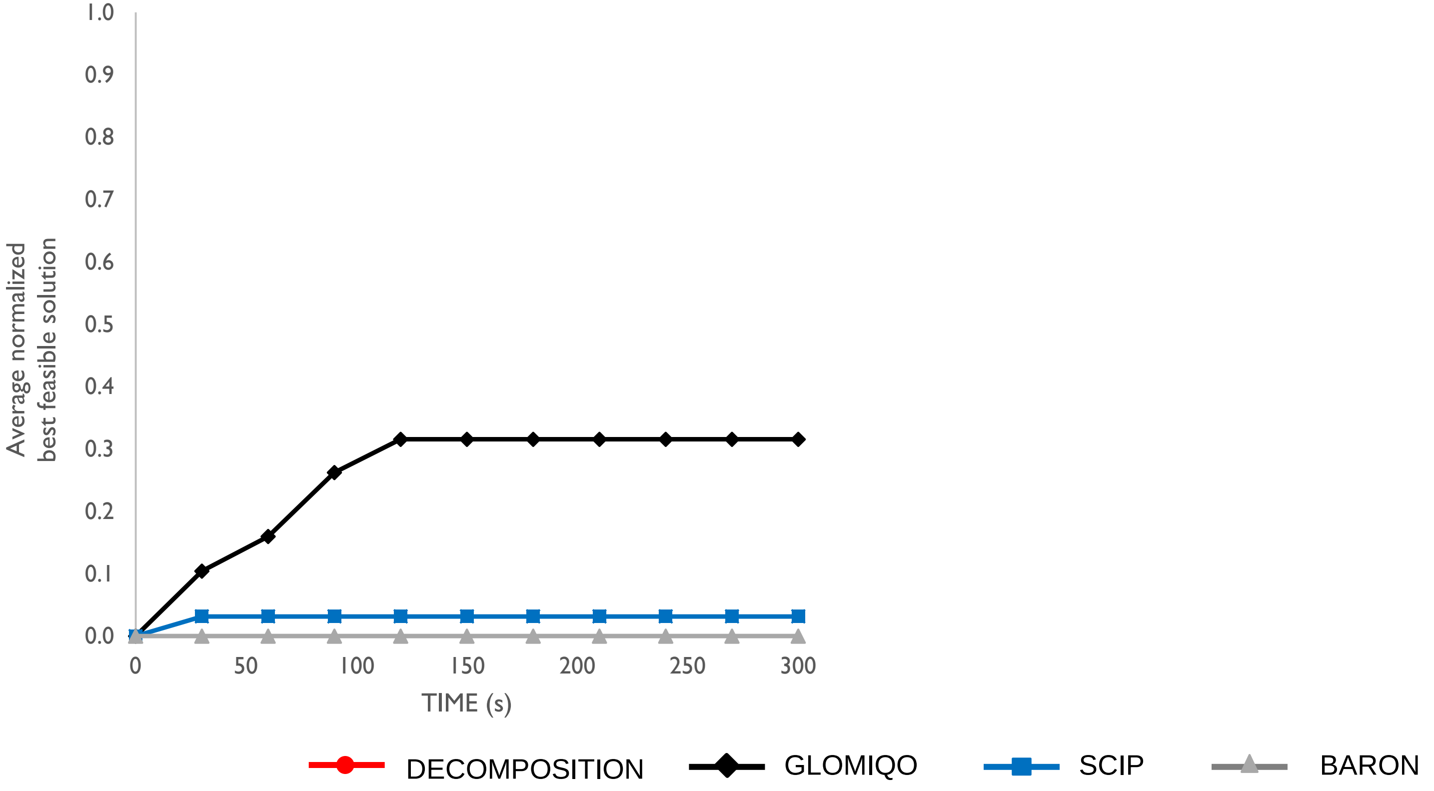
- 18 randomly generated instances
- 3 – 4 time periods, 2 – 10 qualities, 4 – 12 blending tanks



Results Large Instances

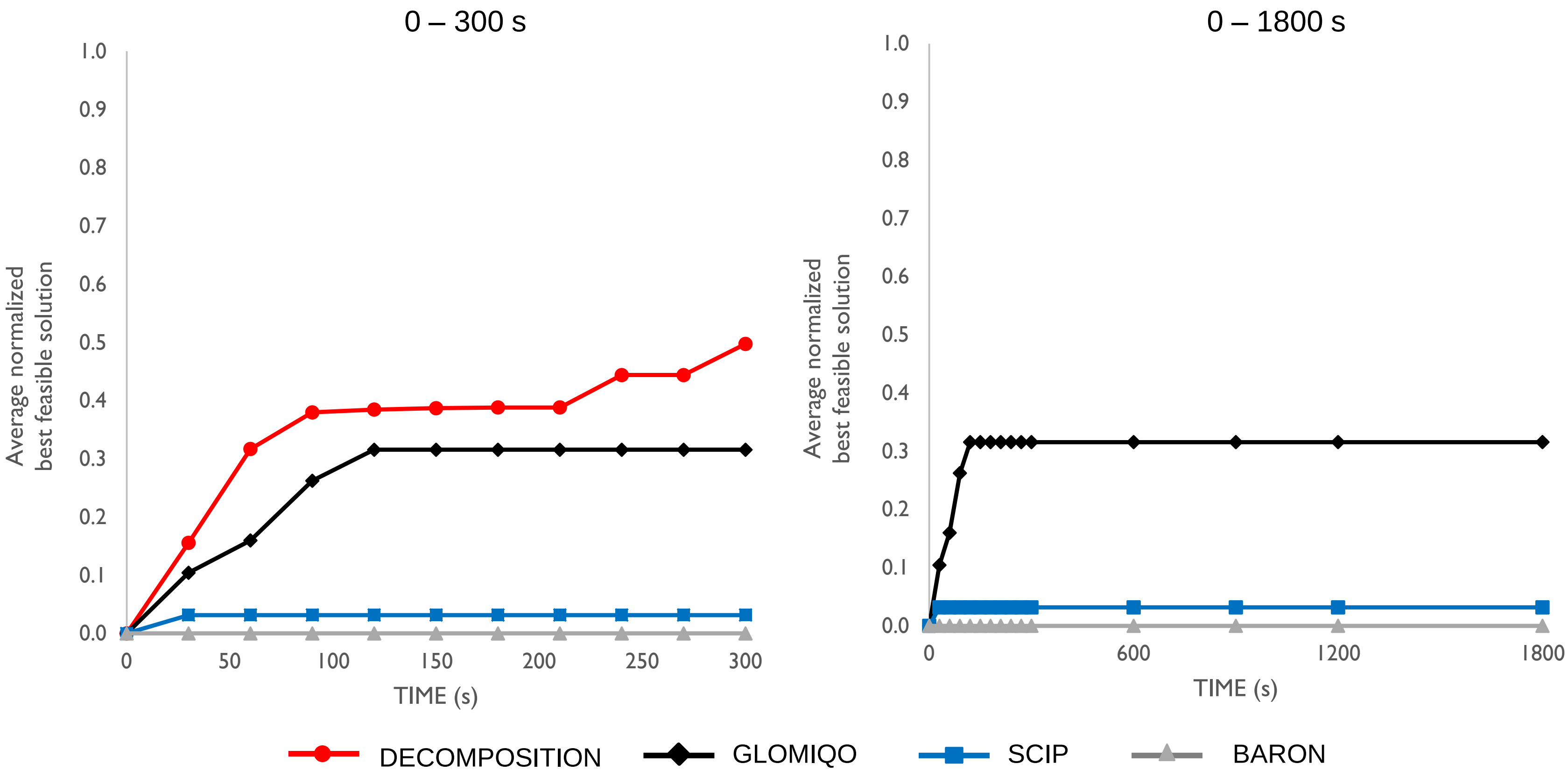
- 18 randomly generated instances
- 4 – 12 time periods, 6 – 10 qualities, 4 – 16 blending tanks

0 – 300 s



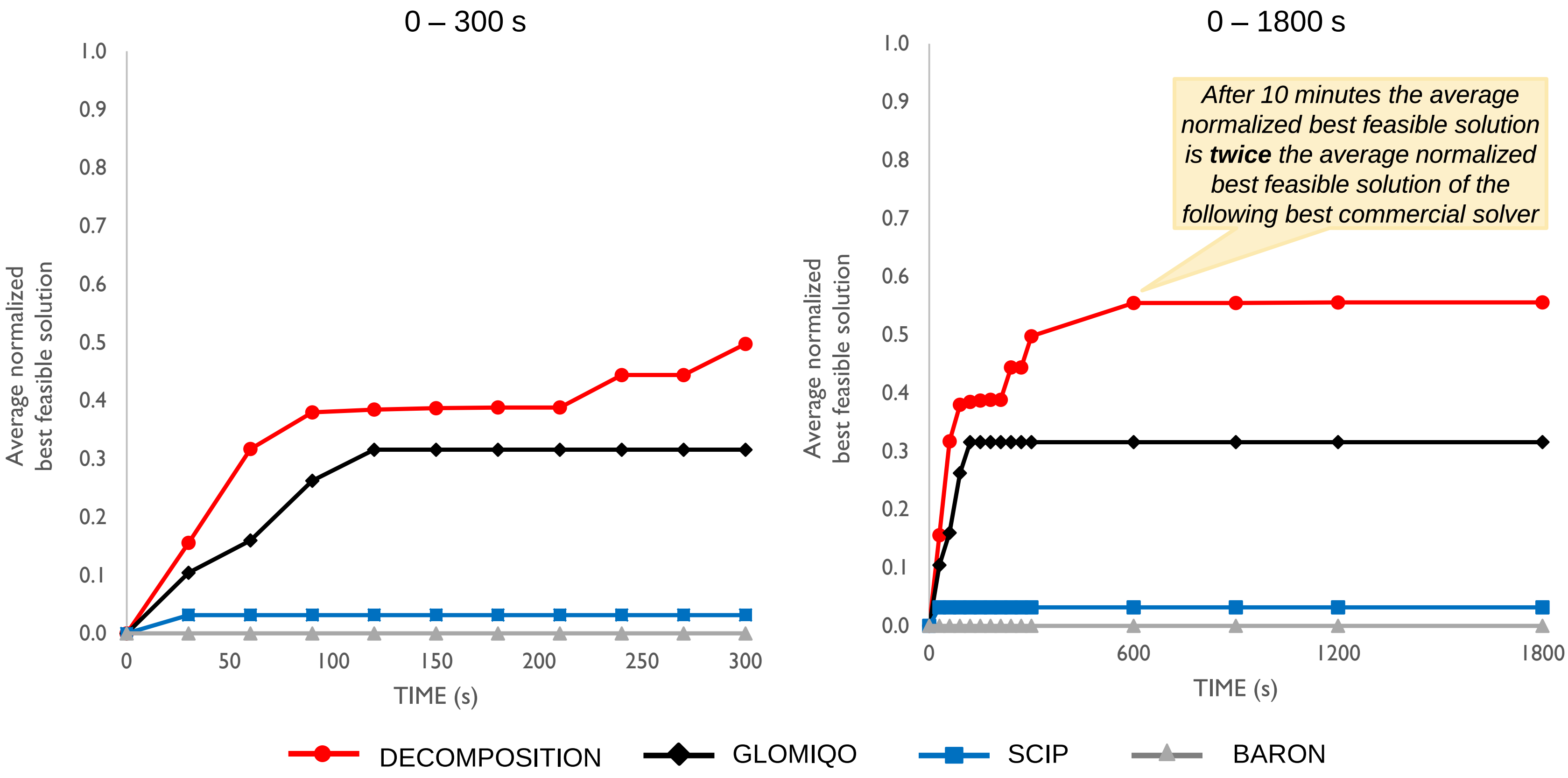
Results Large Instances

- 18 randomly generated instances
- 4 – 12 time periods, 6 – 10 qualities, 4 – 16 blending tanks



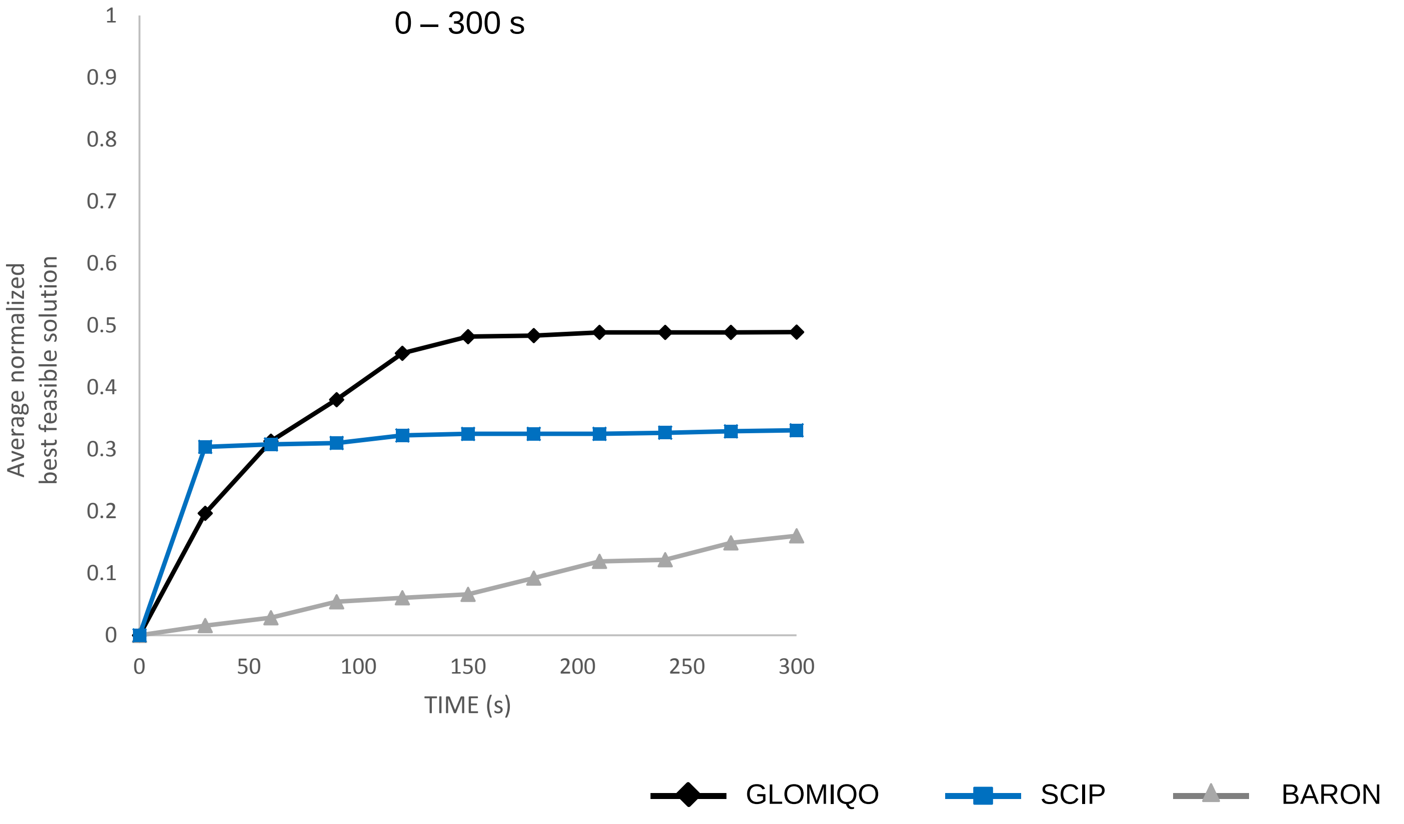
Results Large Instances

- 18 randomly generated instances
- 4 – 12 time periods, 6 – 10 qualities, 4 – 16 blending tanks



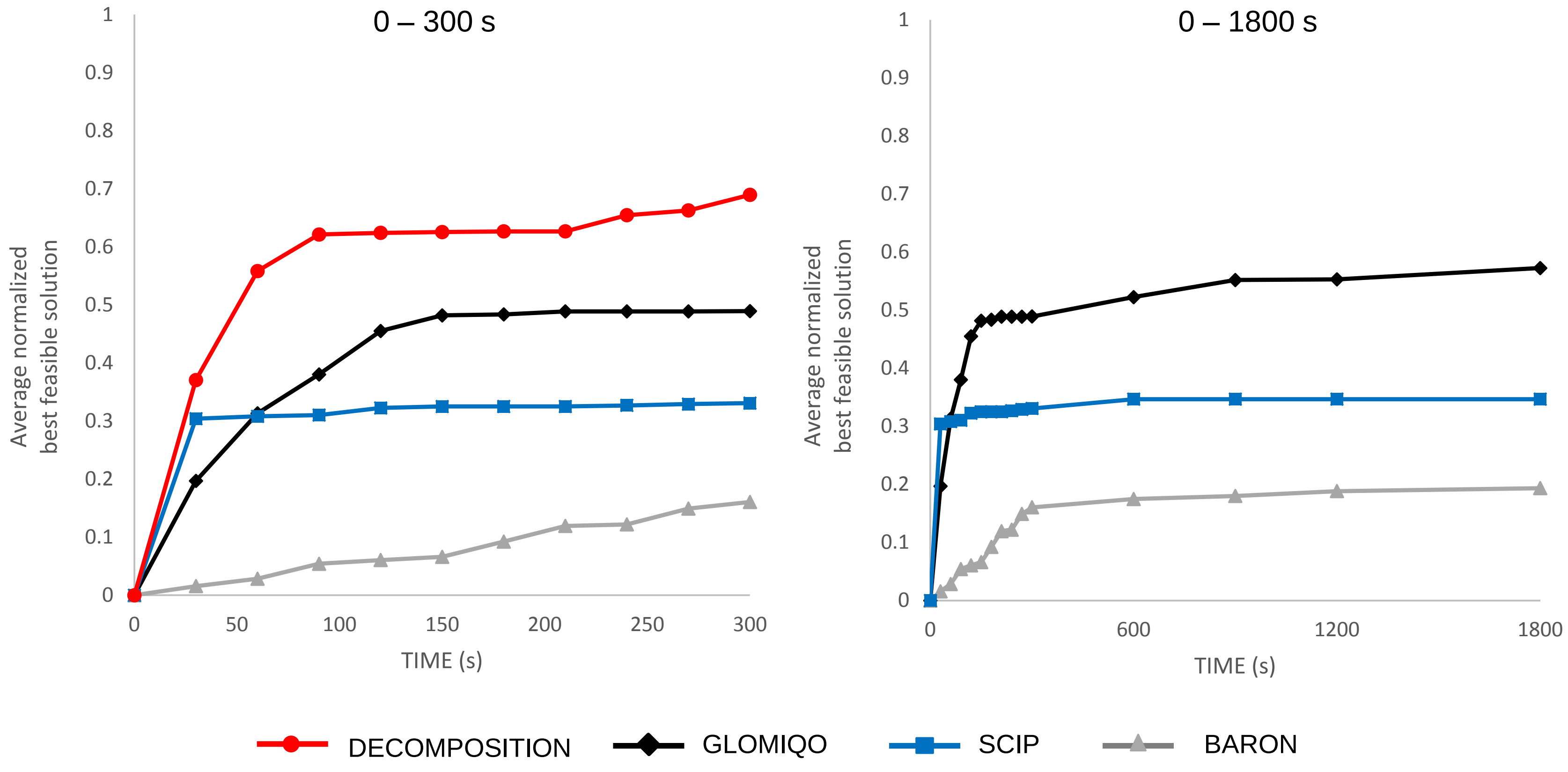
Results All Instances

- 36 randomly generated instances
- 3 – 12 time periods, 2 – 10 qualities, 4 – 16 blending tanks



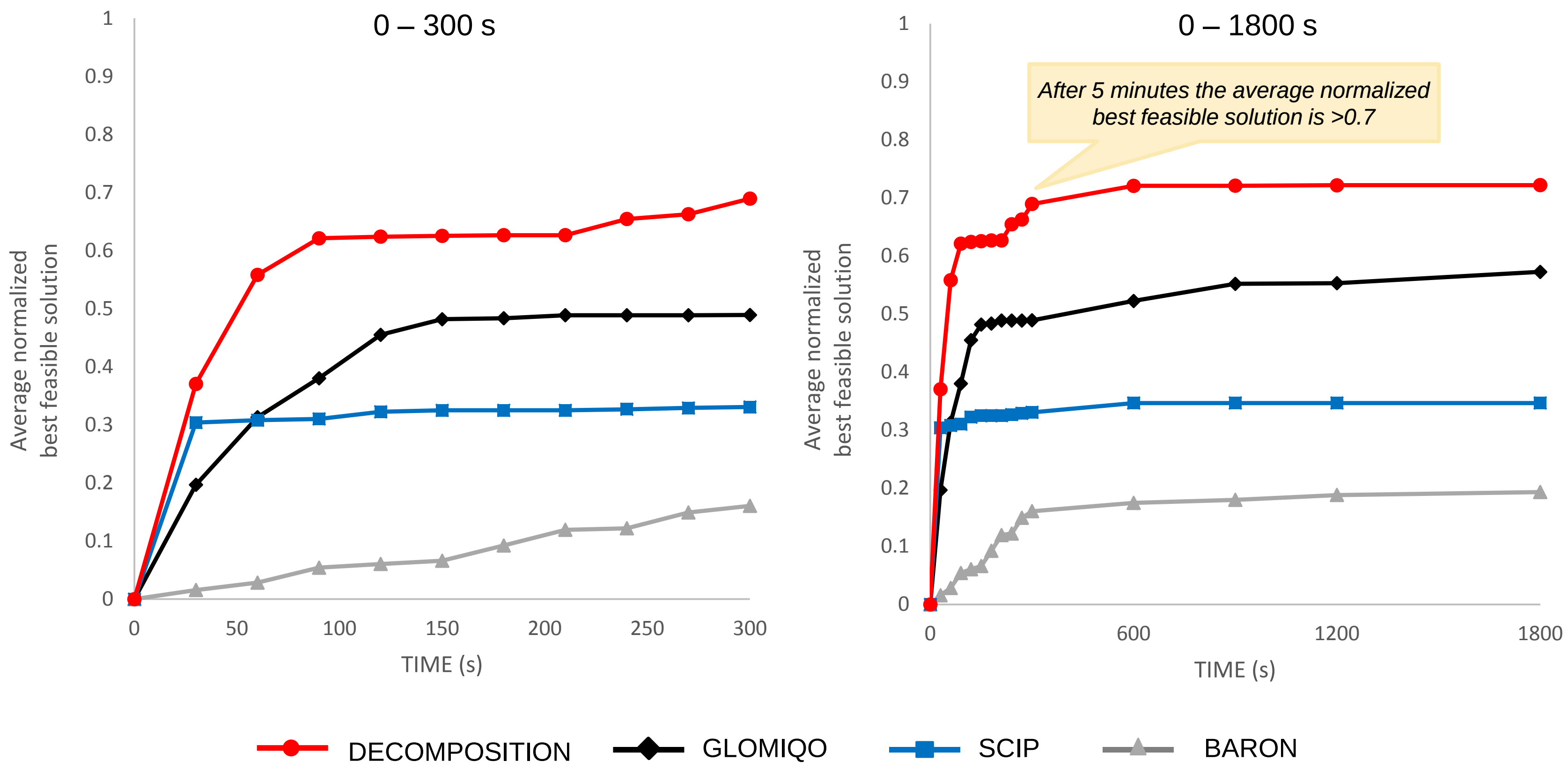
Results All Instances

- 36 randomly generated instances
- 3 – 12 time periods, 2 – 10 qualities, 4 – 16 blending tanks



Results All Instances

- 36 randomly generated instances
- 3 – 12 time periods, 2 – 10 qualities, 4 – 16 blending tanks



The algorithm performs better than state-of-the-art MINLP commercial solvers

Good MILP approximation and decomposition allow finding good solutions in first iteration

Instance	Instance: 0-1 vars	Instance: Bilinear terms	First MINLP: 0-1 vars	First MINLP: Bilinear terms	First iteration (normalized[1]): UB	First iteration (normalized[1]): LB	First iteration (normalized[1]): Time (s)
Group 1	114	195	30	72	1.07	0.94	14.5
Group 2	235	428	63	132	[illegible]	[illegible]	[illegible]
Group 3	539	1071	152	516	1.10	0.69	[illegible]
Group 4	988	1335	223	580	[illegible]	[illegible]	79.7
Group 5	1524	1940	305	446	1.06	0.50	95.4
Group 6	2736	3200	494	1089	[illegible]	0.48	[illegible]

Increase size

~65% fewer bilinear terms

~55% fewer bilinear terms

~75% fewer bilinear terms

70%-80% fewer 0-1 variables

Feasible solution found in less than a minute

Very good solution after 1st iteration

Good solution after 1st iteration

Feasible solution found in less than a two minute

Not as good but at least feasible solution found after 1st iteration

Almost 5 minutes for large instances

1. Normalized to best known solution

To wrap up

Propose an alternative formulation based on GDP

- Blending/Splitting tanks

Decomposition algorithm that simplifies the search for feasible solutions

- Solving smaller MINLPs with fewer 0-1 variables and bilinear terms
- “Guided” by an MILP relaxation of the problem

Tested the approach in randomly generated instances

- Increase problem sizes to match industrial applications

Generate “good” solutions fast

Acknowledgments

Dimitri J. Papageorgiou and Myun-Seok Cheon from ExxonMobil

Thank you