





### Generalized Disjunctive Programming: Helping Creative Researchers Develop Efficient Models Systematically

Pedro M. Castro

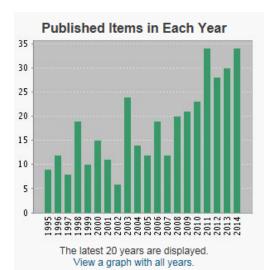


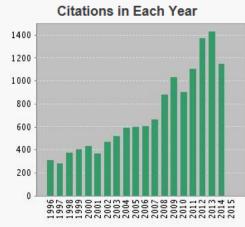




#### Ignacio's citation report







The latest 20 years are displayed. View a graph with all years.

Results found:	460
Sum of the Times Cited [?]:	14855
Sum of Times Cited without self-citations [?]:	12531
Citing Articles [?]:	6019
Citing Articles without self-citations [?]:	5612
Average Citations per Item [?]:	32.29
h-index [?] :	64

2011 2012 2013 2014 2015 Total Average

		- ◀	2012	2010	2011	<b>&gt;</b>	70141	Citations per Year
	se the checkboxes to remove individual items from this Citation Report restrict to items published between 1900 v and 2015 v Go	1108	1378	1432	1152	4	14855	412.64
<u> </u>	AN OUTER-APPROXIMATION ALGORITHM FOR A CLASS OF MIXED-INTEGER NONLINEAR PROGRAMS  By: DURAN, MA; GROSSMANN, IE MATHEMATICAL PROGRAMMING Volume: 36 Issue: 3 Pages: 307-339 Published: DEC 1986	17	38	28	28	0	432	14.90
_ 2.	A COMBINED PENALTY-FUNCTION AND OUTER-APPROXIMATION METHOD FOR MINLP OPTIMIZATION  By: VISWANATHAN, J; GROSSMANN, IE  COMPUTERS & CHEMICAL ENGINEERING Volume: 14 Issue: 7 Pages: 769-782 Published: JUL 1990	15	21	21	11	0	393	15.72
_ 3.	SIMULTANEOUS-OPTIMIZATION MODELS FOR HEAT INTEGRATION .2. HEAT-EXCHANGER NETWORK SYNTHESIS  By: YEE, TF; GROSSMANN, IE COMPUTERS & CHEMICAL ENGINEERING Volume: 14 Issue: 10 Pages: 1165-1184 Published: OCT 1990	25	27	35	31	0	329	13.16
_ 4.	A STRUCTURAL OPTIMIZATION APPROACH IN PROCESS SYNTHESIS .2. HEAT-RECOVERY NETWORKS  By: PAPOULIAS, SA; GROSSMANN, IE  COMPUTERS & CHEMICAL ENGINEERING Volume: 7 Issue: 6 Pages: 707-721 Published: 1983	15	19	20	15	0	294	9.19
<u> </u>	State-of-the-art review of optimization methods for short-term scheduling of batch processes  By: Mendez, Carlos A.; Cerda, Jaime; Grossmann, Ignacio E.; et al.  COMPUTERS & CHEMICAL ENGINEERING Volume: 30   Issue: 6-7   Pages: 913-946   Published: MAY 15 2006	35	44	38	31	0	281	31.22

#### Impact of my publications with Ignacio



GROSSMANN IE (460)
CABALLERO JA (31)

MARTIN M (26)
CASTRO PM (18)

BIEGLER LT (16)

KRAVANJA Z (15)

My contribution to Ignacio's h-index (64)

■ 88.	Two new continuous-time models for the scheduling of multistage batch plants with sequence dependent changeovers  By: Castro, Pedro M.; Grossmann, Ignacio E.; Novais, Augusto Q. INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH Volume: 45   Issue: 18   Pages: 6210-6226   Published: AUG 30 2006	13	5	4	5	0	51	5.67
91.	New continuous-time MILP model for the short-term scheduling of multistage batch plants  By: Castro, PM; Grossmann, IE  INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH Volume: 44   Issue: 24   Pages: 9175-9190   Published: NOV 23 2005	8	5	3	3	0	50	5.00

– Zero! Solid paper!

- Maybe we have just a few joint papers?
  - False! I am #3 in co-authors list
- How about Ignacio's impact on my papers?

	•							
<u> </u>	Simple continuous-time formulation for short-term scheduling of batch and continuous processes  By: Castro, PM; Barbosa-Povoa, AP; Matos, HA; et al.  INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH Volume: 43 Issue: 1 Pages: 105-118 Published: JAN 7 2004	9	12	4	5	0	88	8.00
_ 2.	An improved RTN continuous-time formulation for the short-term scheduling of multipurpose batch plants  By: Castro, P; Barbosa-Povoa, APFD; Matos, H  INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH Volume: 40 Issue: 9 Pages: 2059-2068 Published: MAY 2 2001	5	3	5	5	0	84	6.00
☐ 3.	Improvements for mass-exchange networks design  By: Castro, P; Matos, H; Fernandes, MC; et al.  CHEMICAL ENGINEERING SCIENCE Volume: 54 Issue: 11 Pages: 1649-1665 Published: JUN 1999	5	5	9	2	0	63	3.94

- My top 3 papers? Before I met him!

#### My research work with Ignacio



- First met him in 2004
  - ESCAPE-14, 16-19 May, Portugal
- Visiting researcher to CMU
  - Sep 2004 Jul 2005
    - Scheduling of single & multistage batch plants
      - Continuous-time, Multiple time grids, Constraint Programming, Hybrid MILP/CP
  - Ago-Dec 2008
    - Scheduling of batch & continuous plants
      - Time-dependent electricity costs, Decomposition methods, Dinkelbach algorithm
  - Oct-Nov 2011
    - Multiparametric Disaggregation Technique (lower bound)
    - Development of continuous-time models from GDP
  - Oct-Nov 2013
    - Global optimal scheduling of crude oil blending operations
      - Planning & Scheduling I, Thursday, 1:33 PM, Hilton 406-407



#### Heuristics for efficient MILP models



- Amongst valid choices pick exactly one (exclusive OR)
  - $-\sum_{i,i\neq j} y_{i,j} = 1 \ \forall j \qquad \sum_{j,i\neq j} y_{i,j} = 1 \ \forall i$ 
    - Traveling salesman problem (one arrival & departure from each city)
- Although they look similar
  - Capacity constraints are good
    - $x_i \leq My_i \ \forall i$
  - Big-M constraints are bad
    - $x_i x_{i'} \le M(1 y_i) \ \forall i, i' > i$
- Adding summations makes things tighter

$$- T_{t+1} - T_t \ge \frac{\overline{\xi}_{i,t,t+1}}{\rho_i^{max}} \ \forall i,t \quad \Box \rangle \quad T_{t+1} - T_t \ge \sum_i \frac{\overline{\mu}_{r,i}\overline{\xi}_{i,t,t+1}}{\rho_i^{max}} \ \forall r,t$$

- Timing constraints by equipment unit r rather than task i (Castro et al. 2004)
- Excess resource balances (Pantelides, 1994)

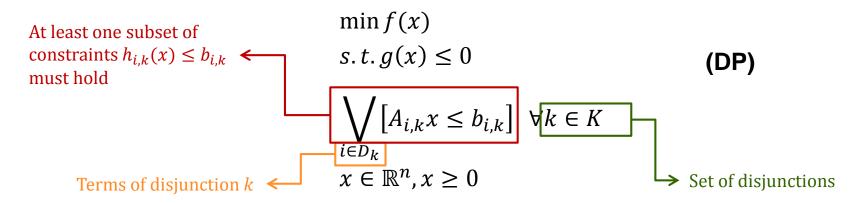
	RMIP	Solution	CPUs
Before	7273	2601	52.2
After	2689	2601	15.6
Before	7361	2620	200,652
After	2695	2638	1913

## Generalized Disjunctive Programming: Systematic Modeling Framework to Derive MILPs

#### Disjunctive Programming (Balas, 1979)



- Most natural & straightforward way of stating problems involving logical conditions
- Any mixed-integer program can be stated as a DP, usually in more than one way
- Various formulations may give rise to linear relaxations of varying strengths
  - Affects computational performance

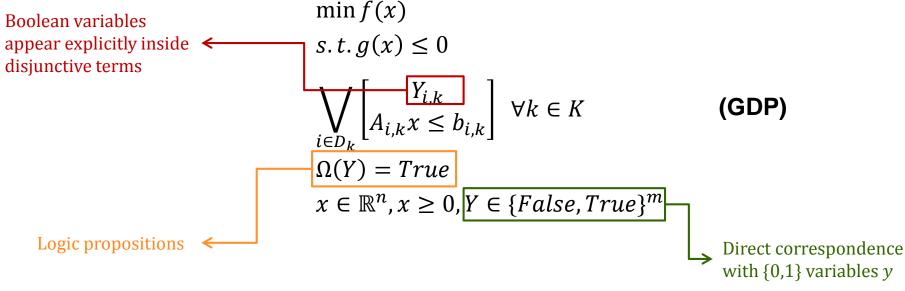


No 0-1 variables explicitly included in the model

#### Generalized Disjunctive Programming



- Logic-based modelling framework (Raman & Grossmann, 1994)
  - 220 citations, #8 (web of Science)
- Adds Boolean variables and logic propositions
  - Selection of a given term in a disjunction may affect other constraints
    - Chemical process synthesis (Raman & Grossmann, 1991)



#### Reformulation of a GDP into MILP



- Disjunctions (Balas, 1985)
  - Big-M
    - Simplest form but yields poor relaxations

$$A_{i,k}x \le b_{i,k} + M_{i,k}(1 - y_{i,k}) \ \forall k \in K, i \in D_k$$

Tightest big-M parameters

$$M_{i,k} = \max\{A_{i,k}x - b_{i,k}: 0 \le x^L \le x \le x^U\} \ \forall k \in K, i \in D_k$$

- Convex hull
  - At least as tight as big-M but increases problem size and is much harder

$$A_{i,k}\hat{x}_{i,k} \leq b_{i,k}y_{i,k} \ \forall k \in K, i \in D_k$$

$$\xrightarrow{\text{Tighter}} \hat{x}_{i,k}^L y_{i,k} \leq A_{i,k}\hat{x}_{i,k} \leq \hat{x}_{i,k}^U y_{i,k} \ \forall k \in K, i \in D_k$$

 $x = \sum_{i \in D_k} \widehat{x}_{i,k} \quad \forall k \in K$ 

Disaggregated variables (new set)

Common constraint

$$\sum_{i \in D_k} y_{i,k} \ge 1 \ \forall k \in K$$

- Logic propositions
  - Replace with linear inequalities (Clocksin & Mellish, 1981)

#### Remarks about big-M way of modeling



- Used extensively by many researchers
  - Avoids bilinear terms

$$IF \ y_{i,k} = 1 \ THEN \ A_{i,k} x \le b_{i,k}$$



$$A_{i,k} x y_{i,k} \le b_{i,k} y_{i,k}$$

Holds true for  $y_{i,k} = 0$ regardless of x

Worst 
$$A_{i,k}xy_{i,k} \le b_{i,k}y_{i,k}$$
 for  $y_{i,k}$  regard of  $A_{i,k}x \le b_{i,k} + M_{i,k}(1-y_{i,k})$ 

- Few bother to calculate  $M_{i,k}$  (global value M used instead)
  - Output from big-M reformulation might not be a big-M constraint
    - Example from scheduling with multiple time grids (Castro & Grossmann, 2012)

$$\bigvee_{\overline{i}} \begin{bmatrix} y_{i,k} \\ x_{k+1} - x_k \ge p_i \\ x_k \ge r_i \end{bmatrix} \forall k \quad \square$$



$$x_{k+1} - x_k \ge p_i - M_{i,k}^1 (1 - y_{i,k}) \, \forall i, k$$
  
 $x_k \ge r_i - M_{i,k}^2 (1 - y_{i,k}) \, \forall i, k$ 



$$x_{k+1} - x_k \ge p_i \cdot y_{i,k} \forall i, k$$
$$x_k \ge r_i \cdot y_{i,k} \ \forall i, k$$

But we can infer that

$$M_{i,k}^1 = \max \{x_k - x_{k+1} + p_i : x_k - x_{k+1} \le 0\} = p_i$$

$$M_{i,k}^2 = \max\{-x_k + r_i : x_k \ge 0\} = r_i$$

#### Remarks about convex hull reformulation



- Always check if disaggregated variables can be removed
  - Compact or sharp formulation (Jeroslow and Lowe, 1984)
    - Example 1: Modeling a semi-continuous variable
      - Flow in a unit only if the unit is selected from the superstructure

$$\begin{bmatrix} y \\ x^{L} \le x \le x^{U} \end{bmatrix} \bigvee \begin{bmatrix} \neg y \\ x = 0 \end{bmatrix} \quad \Longrightarrow \quad \begin{aligned} x &= \hat{x}^{1} + \hat{x}^{2} \\ x^{L} y \le \hat{x}^{1} \le x^{U} y \\ \hat{x}^{2} &= 0 \cdot (1 - y) \end{aligned} \qquad \Longrightarrow \quad x^{L} y \le x \le x^{U} y$$

Example 2: Scheduling with multiple time grids revisited

$$\bigvee_{\bar{i}} \begin{bmatrix} y_{i,k} \\ x_{k+1} - x_k \ge p_i \\ x_k \ge r_i \end{bmatrix} \forall k$$



3.91

CPUs	Big-M (up to 1 h)	Convex hull	Compact Convex hull
EX6	Suboptimal	123	1.53
EX7	No solution	21.6	1.07
EX8	No solution	80.3	1.80
EX9	No solution	63.3	0.59

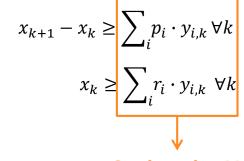
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$$x_{k} = \sum_{i} \hat{x}_{k,i,k} \quad \forall k$$

$$x_{k+1} = \sum_{i} \hat{x}_{k+1,i,k} \quad \forall k$$

$$\hat{\chi}_{k+1,i,k} - \hat{\chi}_{k,i,k} \ge p_i \cdot y_{i,k} \ \forall i,k$$

$$\hat{x}_{k,i,k} \geq r_i \cdot y_{i,k} \ \forall i,k$$



Similar to big-M

$$\sum_{i} y_{i,k} = 1 \ \forall k$$
 Shared by convex hull & compact convex hull



No solution

**EX10** 

#### Advantages of modeling with GDP



- GDP model much easier to understand
  - Constraints
    - In their simplest (linear) form
    - Fewer in number
  - Particularly relevant for complex problems
    - Not uncommon to find research papers featuring MILP models with 50-100 constraints, mostly big-M
      - How can one assess model efficiency?
- Conversion to MILP format can be automated
  - LogMIP for GAMS (Vecchietti & Grossmmann, 2007)
    - Works for very simple cases, cannot handle disjunctions over a set
- Useful guidelines for hands-on approach needed
  - When is it worth to derive convex hull reformulation?



#### Worth to derive convex hull?



General precedence



$$\begin{bmatrix} Y_{t,m,t',m'} \\ Tm_{t,m} + sd_t \leq Tm_{t',m'} \end{bmatrix} \bigvee \begin{bmatrix} \neg Y_{t,m,t',m'} \\ Tm_{\underline{t',m'}} + sd_{t'} \leq Tm_{\underline{t,m}} \end{bmatrix} \forall t,t',m' > m$$

Two variables involved

Similar constraint but the indices have changed

- Answer: No (disaggregated variables with 6 indices)
- Forbid task execution on a given time window

$$\begin{bmatrix} Z_{t,m,tu} \\ Tm_{t,m} + sd_t \leq u_{tu}^L \end{bmatrix} \bigvee \begin{bmatrix} \neg Z_{t,m,tu} \\ Tm_{t,m} \geq u_{tu}^U \end{bmatrix} \forall t,m,tu$$
 Shutdown (t,m) 
$$Z_{t,m,tu} = True$$
 Unavailable period tu 
$$Z_{t,m,tu} = False$$

- Maybe (disaggregated variables with 3 indices)
- Single task per unit

Absolutely, no additional variables and constraints

### Success Cases: Optimization Approaches

#### Relaxation of bilinear term $z_{ij} = x_i x_j$



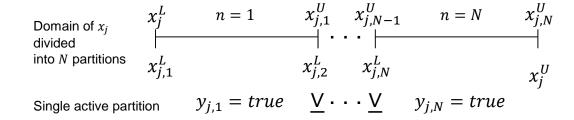
#### Tightest continuous relaxation

McCormick (1976)

# Underestimators $z_{ij} \geq x_i \cdot x_j^L + x_i^L \cdot x_j - x_i^L \cdot x_j^L$ $z_{ij} \geq x_i \cdot x_j^U + x_i^U \cdot x_j - x_i^U \cdot x_j^U$ $z_{ij} \leq x_i \cdot x_j^L + x_i^U \cdot x_j - x_i^U \cdot x_j^L$ $z_{ij} \leq x_i \cdot x_j^U + x_i^L \cdot x_j - x_i^L \cdot x_j^U$ Overestimators

#### Piecewise McCormick envelopes

- Bergamini et al. (2005)



Partition dependent bounds for  $x_i$ 

Disjunction index (n) $\neq$  variables index (i, j)

$$\begin{bmatrix} z_{ij} \geq x_i & x_{j,n}^L + x_i^L \cdot x_j - x_i^L \cdot x_{j,n}^L \\ z_{ij} \geq x_i & x_{j,n}^U + x_i^U \cdot x_j - x_i^U \cdot x_{j,n}^U \\ z_{ij} \leq x_i & x_{j,n}^L + x_i^U \cdot x_j - x_i^U \cdot x_{j,n}^L \\ z_{ij} \leq x_i & x_{j,n}^U + x_i^L \cdot x_j - x_i^U \cdot x_{j,n}^U \\ x_{j,n}^L \leq x_j \leq x_{j,n}^U \end{bmatrix} \forall i,j$$

$$x_{i}^{L} \le x_{i} \le x_{i}^{U}$$

$$x_{j,n}^{L} = x_{j}^{L} + (x_{j}^{U} - x_{j}^{L}) \cdot (n-1)/N$$

$$x_{j,n}^{U} = x_{i}^{L} + (x_{i}^{U} - x_{i}^{L}) \cdot n/N$$

#### PCM relaxation of bilinear program



#### MILP is derived from convex hull reformulation

$$\min z^{R} = f_{0}(x) = \sum_{(i,j) \in BL} a_{ij0} w_{ij} + h_{0}(x)$$

$$f_q(x) = \sum_{(i,j) \in BL} a_{ijq} w_{ij} + h_q(x) \le 0 \ \forall q \in Q \setminus \{0\}$$

$$z_{ij} \ge \sum_{n=1}^{N} (\hat{x}_{ijn} \cdot x_{jn}^{L} + x_{i}^{L} \cdot \hat{x}_{jn} - x_{ijn}^{L} \cdot x_{jn}^{L} \cdot y_{jn})$$

$$z_{ij} \ge \sum_{n=1}^{N} (\hat{x}_{ijn} \cdot x_{jn}^{U} + x_{i}^{U} \cdot \hat{x}_{jn} - x_{ijn}^{U} \cdot x_{jn}^{U} \cdot y_{jn})$$

$$z_{ij} \le \sum_{n=1}^{N} (\hat{x}_{ijn} \cdot x_{jn}^{L} + x_{i}^{U} \cdot \hat{x}_{jn} - x_{ijn}^{U} \cdot x_{jn}^{L} \cdot y_{jn})$$

$$z_{ij} \le \sum_{n=1}^{N} (\hat{x}_{ijn} \cdot x_{jn}^{U} + x_{i}^{L} \cdot \hat{x}_{jn} - x_{ijn}^{L} \cdot x_{jn}^{U} \cdot y_{jn})$$

$$x_{i} = \sum_{n=1}^{N} \hat{x}_{ijn}$$
Sumn disagger

$$x_{j} = \sum_{n=1}^{N} \hat{x}_{jn}$$

$$\sum_{n=1}^{N} y_{jn} = 1$$

$$\forall \{j | (i,j) \in BL\}$$

Summation eliminates the need for disaggregated variables linked to  $z_{ij}$ 

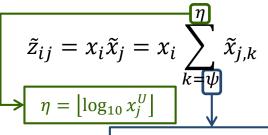
$$(i,j) \in BL \qquad x_{jn}^{L} = x_{j}^{L} + \frac{(x_{j}^{U} - x_{j}^{L}) \cdot (n-1)}{N} \\ x_{jn}^{U} = x_{j}^{L} + \frac{(x_{j}^{U} - x_{j}^{L}) \cdot n}{N} \\ x_{in}^{L} \cdot y_{in} \le \hat{x}_{in} \le x_{in}^{U} \cdot y_{in}$$
 \rightarrow \{j \left| (i,j) \in BL\}, n \in \{1, \ldots, N\}

$$x_i^L \cdot y_{jn} \le \hat{x}_{ijn} \le x_i^U \cdot y_{jn} \ \forall \ (i,j) \in BL, n \in \{1, \dots, N\}$$
$$x^L \le x \le x^U$$
$$x \in \mathbb{R}^m$$
$$y_{jn} \in \{0,1\} \ \forall \ \{j | (i,j) \in BL\}, n \in \{1, \dots, N\}$$

#### Bilinear term approximation $\tilde{z}_{ij} \approx z_{ij} = x_i x_j$

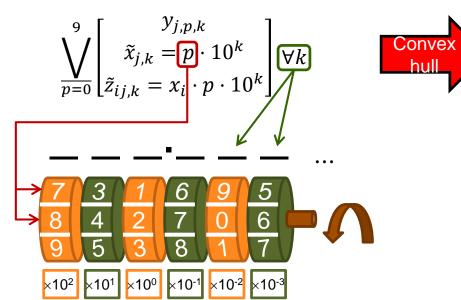


Multiparametric disaggregation (Teles et al. 2013)



MDT discretizes domain of variable  $x_i$  up to a certain accuracy

Defines accuracy level



#### Complete MILP formulation

$$\hat{z}_{ij} = \sum_{k} \sum_{p} \hat{x}_{i,p,k} \cdot p \cdot 10^{k}$$

$$\hat{z}_{ij} = \sum_{k} \sum_{p} \hat{x}_{i,p,k} \cdot p \cdot 10^{k}$$

$$x_{i} = \sum_{p} \hat{x}_{i,p,k} \quad ; \quad \sum_{p} y_{j,p,k} = 1 \quad , \forall k$$

$$x_{i}^{L} \cdot y_{j,p,k} \leq \hat{x}_{i,p,k} \leq x_{i}^{U} \cdot y_{j,p,k} , \forall p, k$$

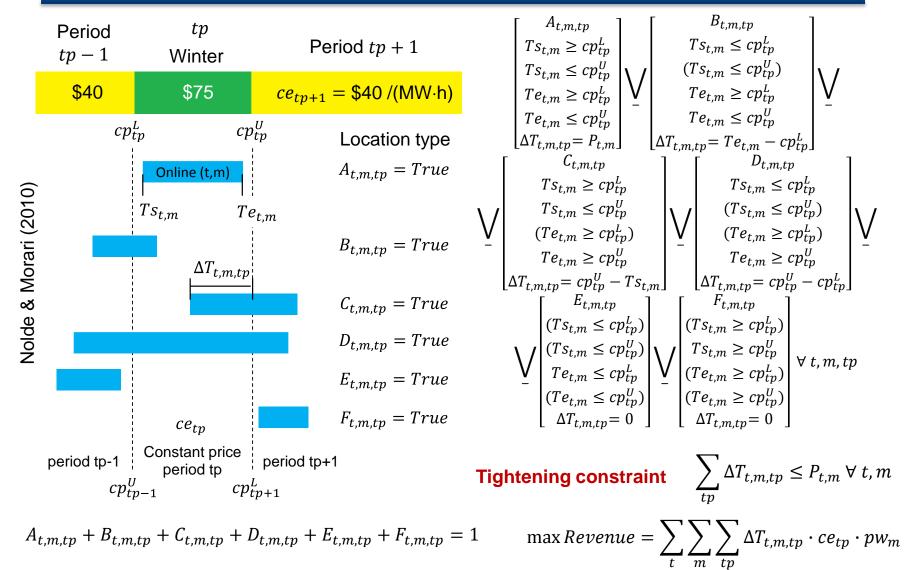
$$x_{j}^{L} \leq \tilde{x}_{j} \leq x_{j}^{U}$$

$$\hat{x}_{i,p,k} \geq 0 \; ; y_{j,p,k} \in \{0,1\}, \forall p, k$$

## Success cases: Industrial scheduling problems dealing with energy

#### Seasonal electricity tariffs in a power plant

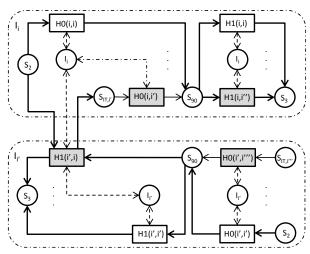




#### Steam sharing in a pulp plant



- Multipurpose plant, single grid, RTN-based approach
  - Superstructure (2001)



- Multistage plant, multiple time grids, GDP-based
  - Embedded disjunctions (2013)
    - Wednesday, 5 PM, Hilton 406-7

$$\bigvee_{i} \begin{bmatrix} Y_{i,t} \\ Te_{t,m} = Ts_{t,m}^{90} + p_{i,m} \\ Z_{i,i',t} \\ Ts_{t,m}^{90} = Ts_{t,m} + p_{i,i'}^{H0} \end{bmatrix} \bigvee_{-} \begin{bmatrix} Z_{i,i,t} \\ Ts_{t,m}^{90} = Ts_{t,m} + p_{i,i}^{H0} \end{bmatrix} \forall m, t$$

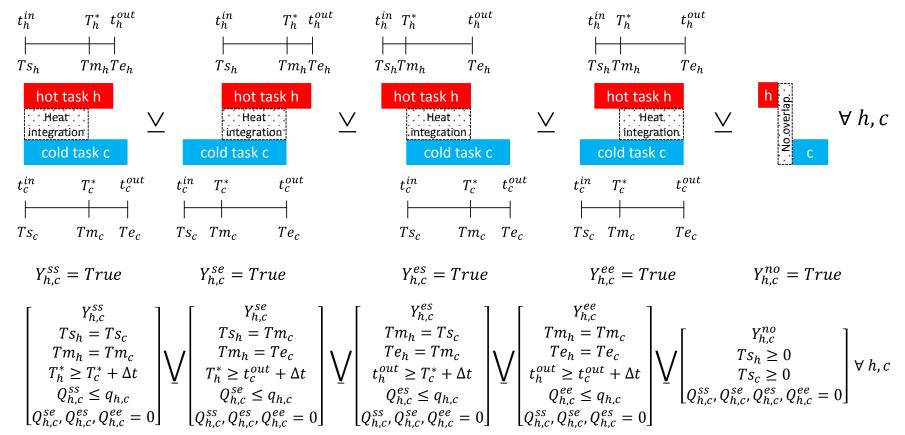
Annanah	Diamete time	Contin	uous-time	Discounts times	Contin	uous-time
Approach	Discrete-time	Single grid	Multiple grids	Discrete-time	Single grid	Multiple grids
Binary variables	33263	2688	79	31583	3584	79
Constraints	30932	3331	132	29372	4435	132
Cycle time H (min)	594	606	594	564	571	564
Total CPU (s)	563	576	0.11	217	25252	0.21



#### Direct heat integration in a batch plant



- Extension of Yee et al. (1990) model for continuous plants
  - Two-stage heating/cooling with matches in parallel
  - Possible interactions between hot & cold stream modelled with GDP



#### Conclusions



- Overview of the basics of linear GDP
- Identification of desired type of disjunctions
  - Leading to sharp (compact) convex hull reformulations
- Examples of global optimization approaches that validate such analysis
  - Piecewise McCormick envelopes
  - Multiparametric Disaggregation Technique
- GDP makes it easier to model complex scheduling problems
  - Alternative formulation with improved performance
    - Orders of magnitude
- Much more about GDP
  - Recent reviews by Grossmann & Trespalacios (2013,14)
    - Further tightening through basic steps
    - · Logic based algorithms for convex GDP
    - Non-convex GDP
- Several research groups worldwide rely on GDP for modeling
  - Many more need to realize how powerful it is!

