Streamlining Life Cycle Assessments: an Emerging Need for **Simplification**

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Janssen Pharmaceutica NV

PDMS – Technical Operations - EHS²

In collaboration with the **Ghent University**

Department of Sustainable Organic Chemistry and Technology

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Introduction – Research group and focus

Introduction: Research group and focus

Ghent University: Department of Sustainable Organic Chemistry and Technology
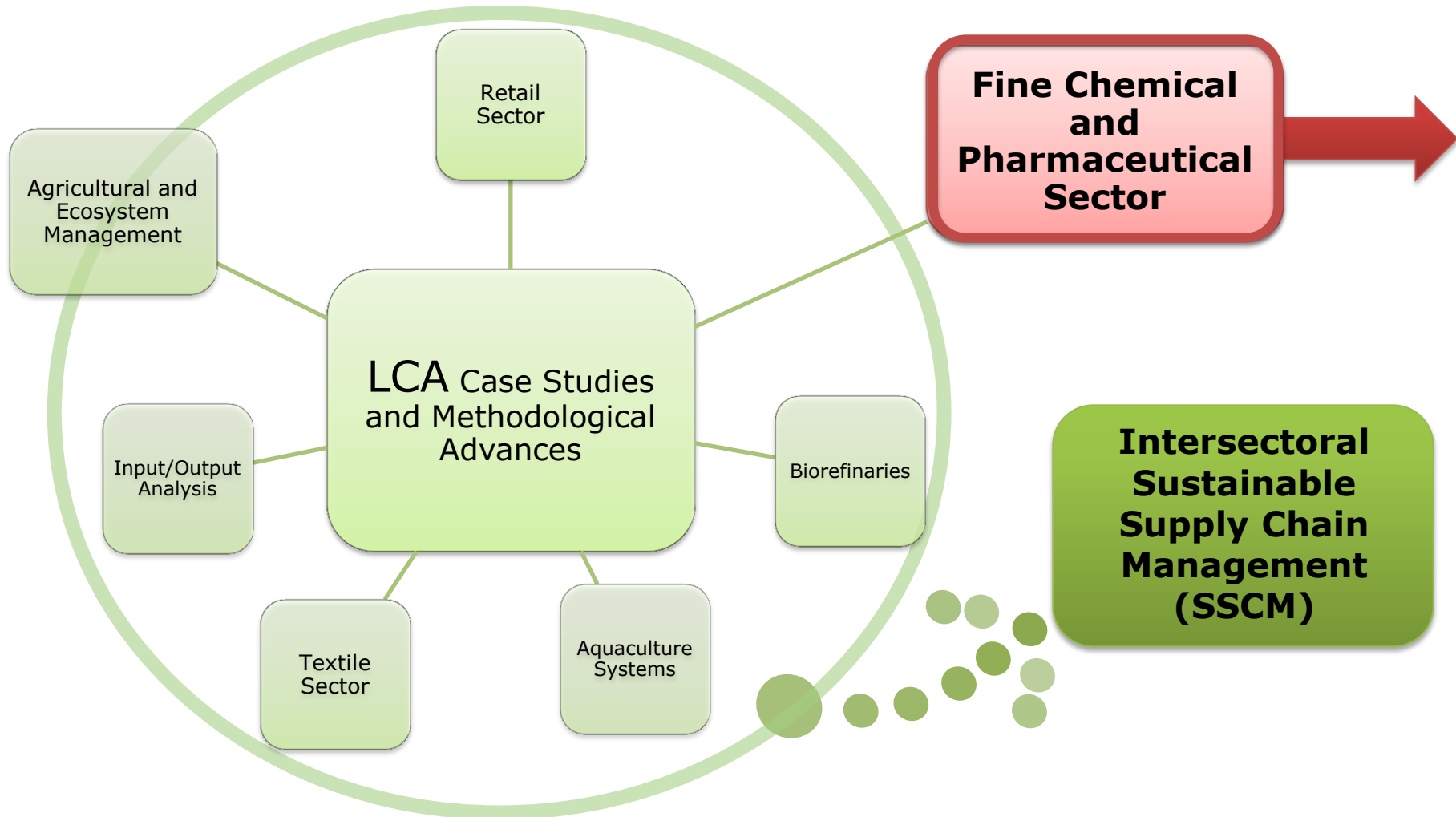

Analytical Environmental Organic Chemistry

Abatement of Organic Micropollutants

Clean Technologies, Process Engineering and LCA

Environmental Resource Management

Introduction: Research group and focus

- Retail Sector
- Agricultural and Ecosystem Management
- LCA Case Studies and Methodological Advances
- Input/Output Analysis
- Textile Sector
- Aquaculture Systems
- Biorefinaries

Fine Chemical and Pharmaceutical Sector

Intersectoral Sustainable Supply Chain Management (SSCM)

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Scope & Objective

Scope & Objective

Life Cycle Based Resource Footprinting of Active Pharmaceutical (API) Synthesis Steps

1) Hotspot Analysis

2) Product Group approach ⟷

Product specific approach

API	# BPRs	# BOs
(A) Domperidone	10	492
(B) Risperidone	7	502
(C) Ketoconazole	8	733
(D) Mitratapide	7	471
(E) Levocabastine	8	641

Methodology

Methodology: hotspot analysis

- **Resource accounting**: How to quantify all different kinds of resources: Energetic & material resources?

→ Exergy Analysis (**EA**) & Exergetic Life Cycle Analysis (**ELCA**, e.g. CEENE Method)
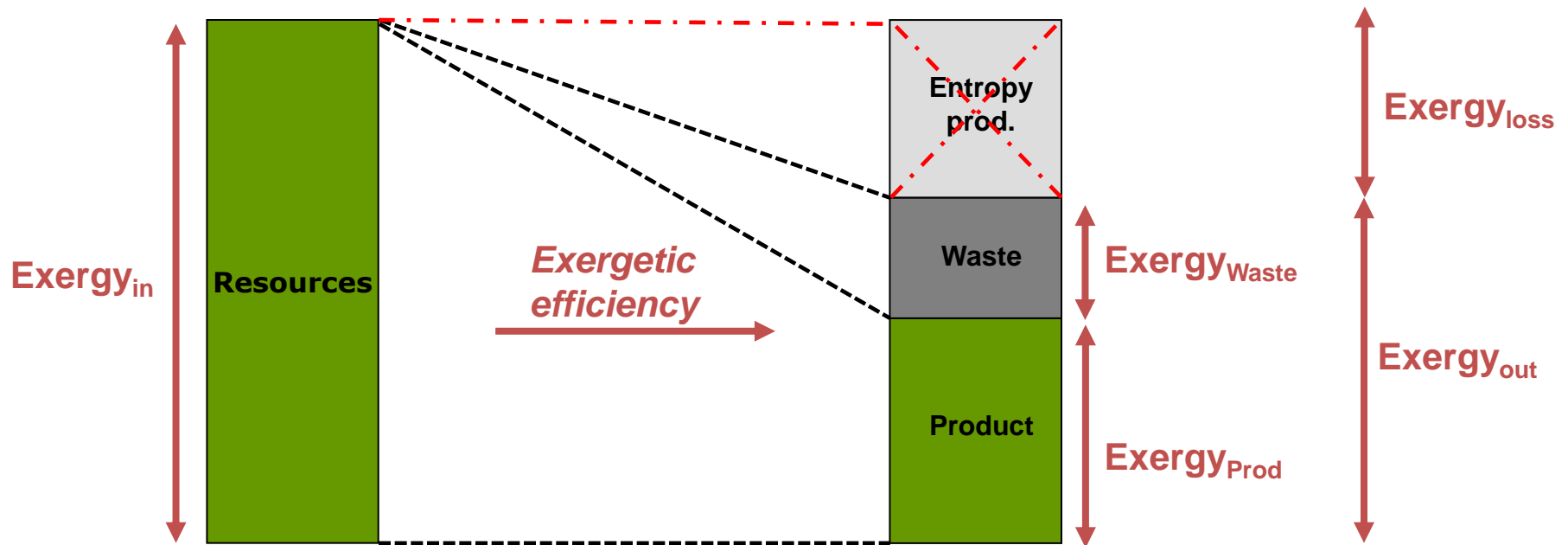
(Dewulf et al., Environ. Sci. Technol., 2008)

Methodology: product group vs product specific

- Average value of cumulative resource consumption data

- Backwards stepwise linear regression modeling:

  - 15 candidate predictor variables, selected based on:
    - Readily availability of data in business ERP systems
    - Expert knowledge

  - 4 predictor variable categories:
    - Process-oriented resource indicators (4)
    - Process operational variables (2)
    - Equipment variables (6)
    - Chemistry variables (3)

Results and Discussion

1) Hotspots identification

Figure: Cumulative exergetic resource consumption (%) for (A) Domperidone (0.92 GJ_{ex}/mole), (B) Risperidone (1.54 GJ_{ex}/mole), (C) Ketoconazole (3.81 GJ_{ex}/mole), (D) Mitratapide (6.59 GJ_{ex}/mole), (E) Levocabastine (8.73 GJ_{ex}/mole). Legend categories: Transport and treatment, Cleaning, Inert gas, Cooling, Heating, Electromechanical, Chemicals.
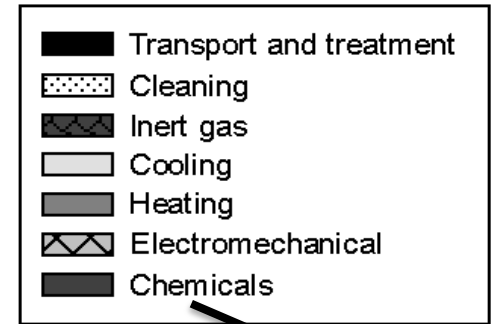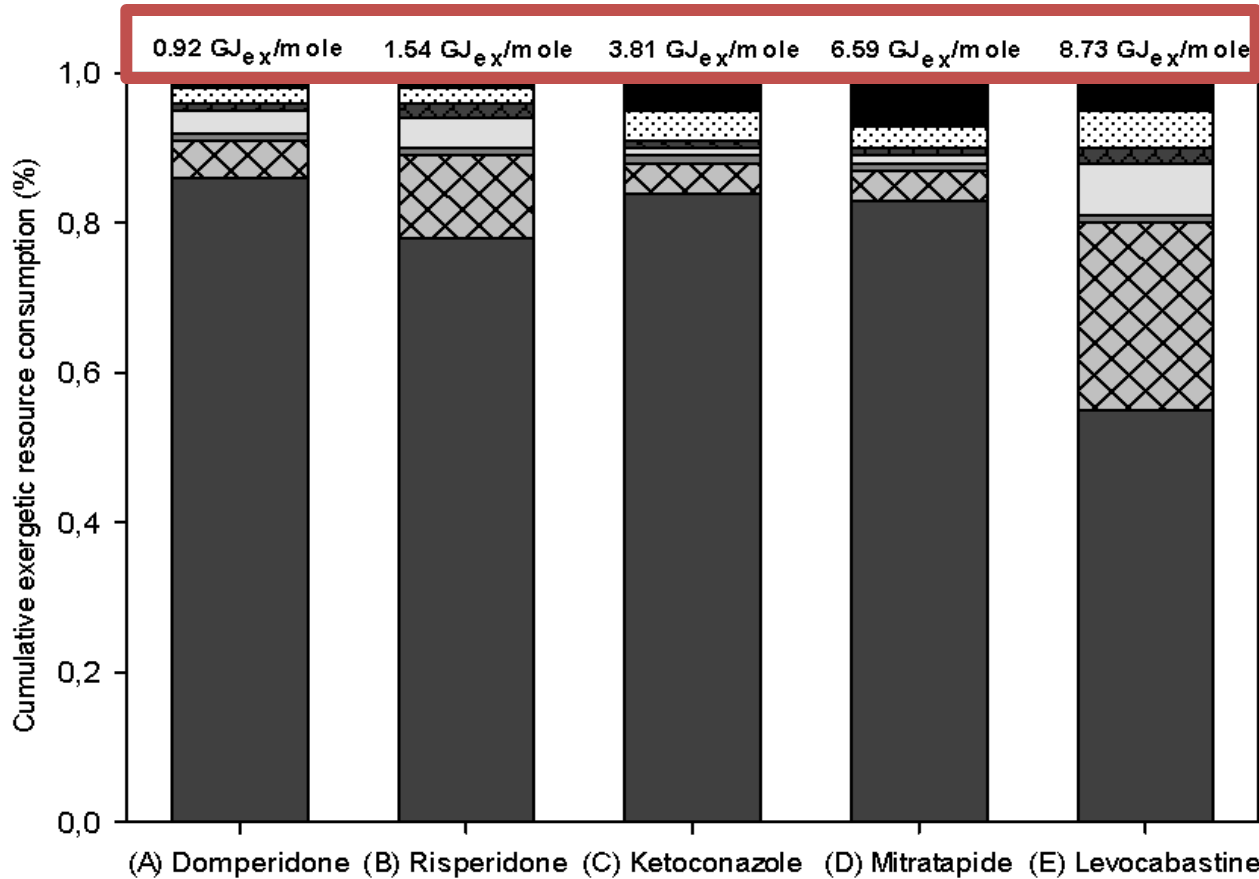
Subdivision of Chemicals
OS: 67.2%
BB: 22.5%
Reagents: 10.2%
Catalysts: 0.1%

De Soete et al., 2014, ES&T

2)

Predicted LOG(CEENE) (kJ$_{ex}$/mole$_{intermediate}$)

Predictor variable: LOG(Organic Solvent)   R² = 0.690
Predictor Variable: LOG(PMI)   R² = 0.663
Predictor Variable: LOG(PMI*MW)   R² = 0.789
Predictor Variable: LOG(Molar Efficiency)   R² = 0.362
Predictor Variable: LOG(Δt)   R² = 0.702
Predictor Variable: LOG(ΔT)   R² = 0.564
Predictor Variable: LOG(# Reactors)   R² = 0.694
Predictor Variable: SQRT(# Filters)   R² = 0.131
Predictor Variable: SQRT(# Tanks)   R² = 0.075
Predictor Variable: SQRT(# Centrifuges)   R² = 0.568
Predictor Variable: SQRT(# Dryers)   R² = 0.555
Predictor Variable: LOG(# Fixed Equipment)   R² = 0.545
Predictor Variable: Addition (boolean)   R² = 0.077
Predictor Variable: Substitution (boolean)   R² = 0.002
Predictor Variable: Elimination (boolean)   R² = 0.046

LOG(CEENE) (kJ$_{ex}$/mole$_{intermediate}$)

Selected Predictors:

Organic Solvent use
Molar Efficiency
Δt
ΔT
Reactors

De Soete et al., 2014, ES&T
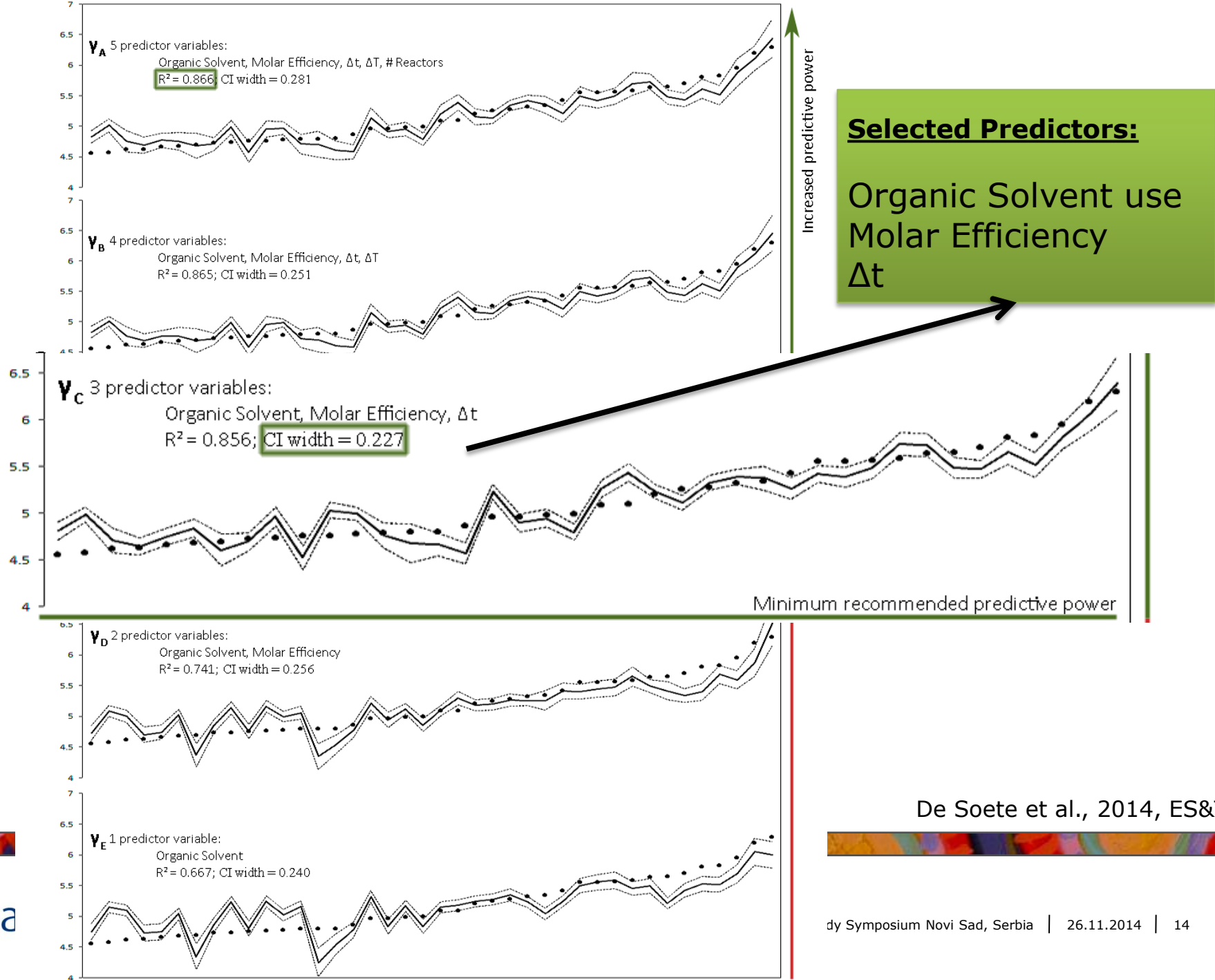
2)

γ_A 5 predictor variables:
Organic Solvent, Molar Efficiency, Δt, ΔT, # Reactors
$R^2 = 0.866$; CI width = 0.281

γ_B 4 predictor variables:
Organic Solvent, Molar Efficiency, Δt, ΔT
$R^2 = 0.865$; CI width = 0.251

γ_C 3 predictor variables:
Organic Solvent, Molar Efficiency, Δt
$R^2 = 0.856$; CI width = 0.227

γ_D 2 predictor variables:
Organic Solvent, Molar Efficiency
$R^2 = 0.741$; CI width = 0.256

γ_E 1 predictor variable:
Organic Solvent
$R^2 = 0.667$; CI width = 0.240

Increased predictive power

Minimum recommended predictive power

Selected Predictors:

Organic Solvent use
Molar Efficiency
Δt

De Soete et al., 2014, ES&T

Research Outlook

Research Outlook

- **Improved data acquisition systems** from sensors, PLCs, etc. to central enterprise data systems (e.g. SAP, Infor LN)

- Relate findings to other impact assessment methods

- Sustainable Supply Chain Management (**SSCM**)

    – It makes little sense to optimise in-house production without a proper procurement policy!! → Coupling organisation's ERP systems

Thank You !

Q/A

Janssen Pharmaceutica
PDMS – Technical Operations - EHS²

Ghent University
Dep. Env. Organic Chemistry and Technology

Wouter.DeSoete@UGent.be