GREEN CHEMISTRY EDUCATION:
TOWARDS A SYSTEMS THINKING APPROACH

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INTRODUCTION (1)

GC TEACHING APPROACH IN OPORTO

STARTED IN

INDUSTRIAL CHEMISTRY & SIMILAR COURSES:

MINDSET OF SYSTEMS THINKING

↓

OBJECTIVES

1 - PRESENT OUR GC TEACHING ACTIVITIES

+

2 - SHOW THE IMPORTANCE OF SYSTEMS THINKING FOR GC

INTRODUCTION (2)

TOPICS

1

EXAMPLES OF “EARLY GC” (< 1990) IN INDUSTRIAL CHEMISTRY

2

DESCRIPTION OF GC IN A SYSTEMS THINKING MINDSET

3

GREENNESS HOLISTIC SYSTEMIC METRICS

4

STRATEGY TO TEACH GC IN THE LABORATORY

GC TEACHING AT OPORTO (1)

2000

SECTIONS ON GC IN 2 COURSES

BSc CHEM ➔ EU BOLOGNA´S BSc & MSc

INDUSTRIAL CHEMISTRY➔INDUSTRIAL GC

(3RD YEAR, 1ST SEM)

IND. ECOLOGY & SUSTAINABILITY ENGINEERING

(4TH YEAR, 2ND SEM)

GC TEACHING AT OPORTO (2)

2005

MSc EDUCATIONAL CHEM. DEGREE

SECONDARY SCHOOL TEACHERS

ONE SEMESTER GC COURSE

WITH LABORATORY ACTIVITIES

SMALL NUMBERS OF STUDENTS

"EARLY GC" (1)

HISTORY OF INDUSTRIAL CHEMISTRY

(18TH CENTURY – 1990)

1

CASES WHERE NEGATIVE ENVIRONMENTAL & HEALTH IMPACTS WERE ELIMINATED:

"EARLY GC" PRACTICED!!!

2

"NEGATIVE" EXAMPLES

(FALSE GREEN PRODUCTS, ETC.)

"EARLY GC" (2)

TABLE 1 - EXAMPLES OF EARLY GC: INDUSTRIAL PROCESSES

EXAMPLE	GREENNESS FEATURES
PROCESS SUBSTITUTION IN SODA MANUFACTURE LEBLANC → SOLVAY	REPLACEMENT OF A VERY POLLUTING PROCESS BY A GREENER ONE
MANUFACTURE OF SULFURIC ACID (LEAD CHAMBER & CONTACT PROCESS)	GREEN SYNTHESIS: CATALYTIC REACTIONS 100% ATOM ECONOMY, PROVIDES ENERGY
EMERGING PETROCHEMICAL INDUSTRY: REFORMING AND CRACKING	CATALYTIC REACTIONS FOR TRANSFORMATION OF RESIDUAL CO-PRODUCTS IN SALABLE PRODUCTS: LOW E-FACTORS

“EARLY GC” (3)

TABLE 1 (CONT) - EXAMPLES OF EARLY GC: PRODUCTS

EXAMPLE	GREENNESS FEATURES
SMOKELESS POWDER	HEALTH & SAFETY INTRINSIC BENIGNITY: SAFE PRODUCT FOR UTILIZERS
MANUFACTURE OF DYNAMITE BY NOBEL (SAFE USE OF NITROGLYCERINE AS AN EXPLOSIVE)	SAFETY OF PRODUCT: FORMULATION TO DECREASE RISKS

"EARLY GC" (4)

TABLE 2 – NEGATIVE EXAMPLES OF EARLY GC

FREONS (CFCs)	FALSE GC: ADVERTISED AS SAFE PRODUTCS, BUT UNEXPECTED SIDE DANGEROUS IMPACTS FOUND LATER
BHOPAL DISASTER	ABANDONMENT OF GC: SUBSTITUTION OF A GREEN BY A DANGEROUS SYNTHETIC PATHWAY

“EARLY GC” (5)

DISCUSSION AS PRELIMINARY MATERIAL

- SMOOTH INTRODUCTION TO GC
- GC IMPLEMENTED IN *INDUSTRIAL SYSTEMS*
- USEFUL KNOWLEDGE FOR STRATEGIC DEVELOPMENT OF GC
- STRESSES THE IMPORTANCE OF SYSTEMS THINKING IN GC

“EARLY GC” (6): LEBLANC ➔ SOLVAY

19^{TH} CENTURY:

EMERGING CHEMICAL INDUSTRY

Na_2CO_3 (“SODA ASH”) MANUFACTURE:

LEBLANC PROCESS ➔ SOLVAY PROCESS

“EARLY GC” (7): LEBLANC ➔ SOLVAY

INDUSTRIAL REVOLUTION

REQUIRED INCREASING AMOUNTS OF

BASIC CHEMICALS

ALKALIS TO BLEACH COTTON

Na_2CO_3

“EARLY GC” (8): LEBLANC → SOLVAY

Na_2CO_3

OBTAINED FROM BIOMASS:

BURNING PLANTS + WATER EXTRACTION

KELP - SCOTLAND

BARILLA - SOUTH SPAIN

RENEWABLE: GREEN PRODUCT!

“EARLY GC” (9): LEBLANC ➔ SOLVAY

1791

INVENTION OF LEBLANC PROCESS

RAW MATERIALS:

SALT + LIMESTONE + COAL + SULFURIC ACID

SYNTHESIS PATHWAY: 2 REACTIONS

LEBLANC + LEAD CHAMBER PROCESS (H_2SO_4):

ORIGIN OF INDUSTRIAL CHEMISTRY

“EARLY GC” (10): LEBLANC ➔ SOLVAY

INDUSTRIAL SUCCESS:

MANY PLANTS BUILT IN FRANCE, UK, …

INCREASE OF THE SCALE OF THE PLANTS

SEVERE ENVIRONMENTAL IMPACTS

DUE TO BYPRODUCTS

"EARLY GC" (11): LEBLANC ➔ SOLVAY

LEBLANC PROCESS

(1) PREPARATION OF SODIUM SULFATE ("SALT CAKE")

$NaCl + H_2SO_4 \rightarrow Na_2SO_4 + 2\ HCl$

TOXIC FUMES

(2) CONVERSION OF THE "SALT CAKE" TO "BLACK ASH"

$Na_2SO_4 + 4\ C + CaCO_3 \rightarrow Na_2CO_3 + CaS + 4\ CO$

$H_2S + SO_2$

(3) EXTRACTION OF Na_2CO_3 WITH H_2O

“EARLY GC” (12): LEBLANC ➔ SOLVAY

DEVASTATING IMPACTS

HCl

HEALTH OF WORKERS

$HCl + H_2S + SO_2$

POPULATION: HEALTH

ENVIRONMENT: VEGETATION, CORROSION, …

“EARLY GC” (13): LEBLANC ➔ SOLVAY

NO ENVIRONMENTALISTS BUT…

“END OF PIPE” MEASURES

1

REMOVAL OF THE “BLACK ASHES” TO OLD MINES

2

ABSORPTION TOWERS FOR RETENTION OF HCl DISCHARGE TO RIVERS

MOVING POLLUTANTS BETWEEN COMPARTMENTS!

"EARLY GC" (14): LEBLANC → SOLVAY

MEASURES

- DIFFICULT TO IMPLEMENT/INOPERATIVE
- EXPENSIVE: EXAMPLE OF POLLUTION COSTS!

ALTERNATIVE SYNTHETIC PATHWAYS SEARCHED

"POLLUTION PREVENTION"

SOLVAY PROCESS (1863)

"EARLY GC" (15): LEBLANC ➔ SOLVAY

SOLVAY PROCESS

(1) BUBBLING OF CO_2 THROUGH NaCl SATURATED WITH NH_3

$$NaCl + NH_3 + CO_2 + H_2O \rightarrow NaHCO_3 + NH_4Cl$$

(2) HEATING OF $NaHCO_3$

$$NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$$

(3) NH_3 RECOVERY

$$2\ NH_4Cl + CaO \rightarrow 2\ NH_3 + CaCl_2 + H_2O$$

INNOVATION:

RECYCLING OF NH_3

(AUXILIARY REAGENT)

INNOVATION: PATHWAY WITHOUT NEGATIVE IMPACTS OF RESIDUES

“EARLY GC” (16): LEBLANC → SOLVAY

SOLVAY PROCESS

- NO SEVERE ENVIRONMENTAL IMPACTS
- TECHNICALLY SIMPLER
- BETTER ECONOMY

AUXILIARY MATERIAL RECOVERED & RECIRCULATED:
NO EMISSION AS POLLUTANT

↓

RECYCLING OF MATERIALS TO SAVE ATOMS
LATER COMMONLY USED IN CHEMICAL INDUSTRY

“EARLY GC” (17): LEBLANC ➔ SOLVAY

SOLVAY PROCESS

EARLY EXAMPLE OF

- DELIBERATE SUCCESSFUL SEARCH OF A NEW SYNTHETIC PATHWAY FOR ELIMINATING ENVIRONMENTAL IMPACTS
- PROACTIVE MEASURES FOR PREVENTING RESIDUES BY RECYCLING

(1^{ST} PRINCIPLE)

"EARLY GC" (18): LEBLANC → SOLVAY

EXAMPLE OF

CONTRIBUTION OF CHEMISTRY TO SUSTAINABLE DEVELOPMENT

A CLEANER TECHNOLOGY → DEFENSE OF THE ENVIRONMENT

CONTRIBUTED AS WELL TO

CHEAP COTTON CLOTHES FOR THE PEOPLE → SOCIETAL GOOD

ECONOMIC DEVELOPMENT → WEALTH CREATION

“EARLY GC” (19): LEBLANC → SOLVAY

SOLVAY PROCESS BETTER THAN LEBLANC PROCESS BUT…

COMPLETE REPLACEMENT SLOW

SOLVAY PROCESS → NEW PLANTS

EXISTENT LEBLANC PLANTS → KEPT WORKING UNTIL THE END OF THE 1st GREAT WAR

USED IN PARALLEL > 40 YEARS

“EARLY GC” (20): LEBLANC ➔ SOLVAY

HOEWELLS (2005):

CASE STUDY

MANAGEMENT OF TECHNOLOGICAL INNOVATION

⬇

SHOWS PRESENT DIFFICULTIES OF PENETRATION OF GC IN INDUSTRY

“EARLY GC” (21): LEBLANC → SOLVAY

RESISTANCE OF THE LEBLANC PROCESS AGAINST A BETTER COMPETITOR?

CAUSES OF TWO TYPES

1

- INVENTION OF PROCESSES FOR RECOVERY OF THE RESIDUES
- MANUFACTURE OF OTHER PRODUCTS

EARLY GC" (22): LEBLANC ➔ SOLVAY

RECOVERY OF RESIDUES FROM THE LEBLANC PROCESS

1 – HCl RECOVERY (AS Cl_2) – MANUFACTURE OF "BLEACHING POWDER" (CaClOCl)

$4\ HCl + MnO_2 \rightarrow Cl_2 + MnCl_2 + 2\ H_2O$

$Cl_2 + Ca(OH)_2 \rightarrow CaClOCl + H_2O$

WITH Mn RECOVERY

$MnCl_2 + Ca(OH)_2 \rightarrow Mn(OH)_2 + CaCl_2$ **(WELDON PROCESS, 1869)**

$Mn(OH)_2 + ½\ O_2 \rightarrow MnO_2 + H_2O$

ALTERNATIVE (GAS PHASE, CATALYST: $CuCl_2$)

$2\ HCl + ½\ O_2 \rightarrow Cl_2 + H_2O$ **(DEACON PROCESS, 1868)**

2 – S RECOVERY (CLAUS-CHANCE PROCESS)

$CaS + CO_2 + H_2O \rightarrow CaCO_3 + H_2S$ **(CHANCE PROCESS, 1882)**

$H_2S + ½\ O_2 \rightarrow S + H_2O$ **(CLAUS PROCESS, 1988)**

EARLY GC" (23): LEBLANC → SOLVAY

PROCESS MODIFIED TO PRODUCE

NaOH ("CAUSTIC SODA")

PROFIT: NaOH > Na_2CO_3

RECYCLING + NEW PRODUCTS:

CONTRIBUTED TO KEEP LEBLANC IN COMPETITION WITH A ETTERPROCESS

EARLY GC" (24): LEBLANC → SOLVAY

INVENTION OF AN

ECO-INDUSTRIAL SYSTEM

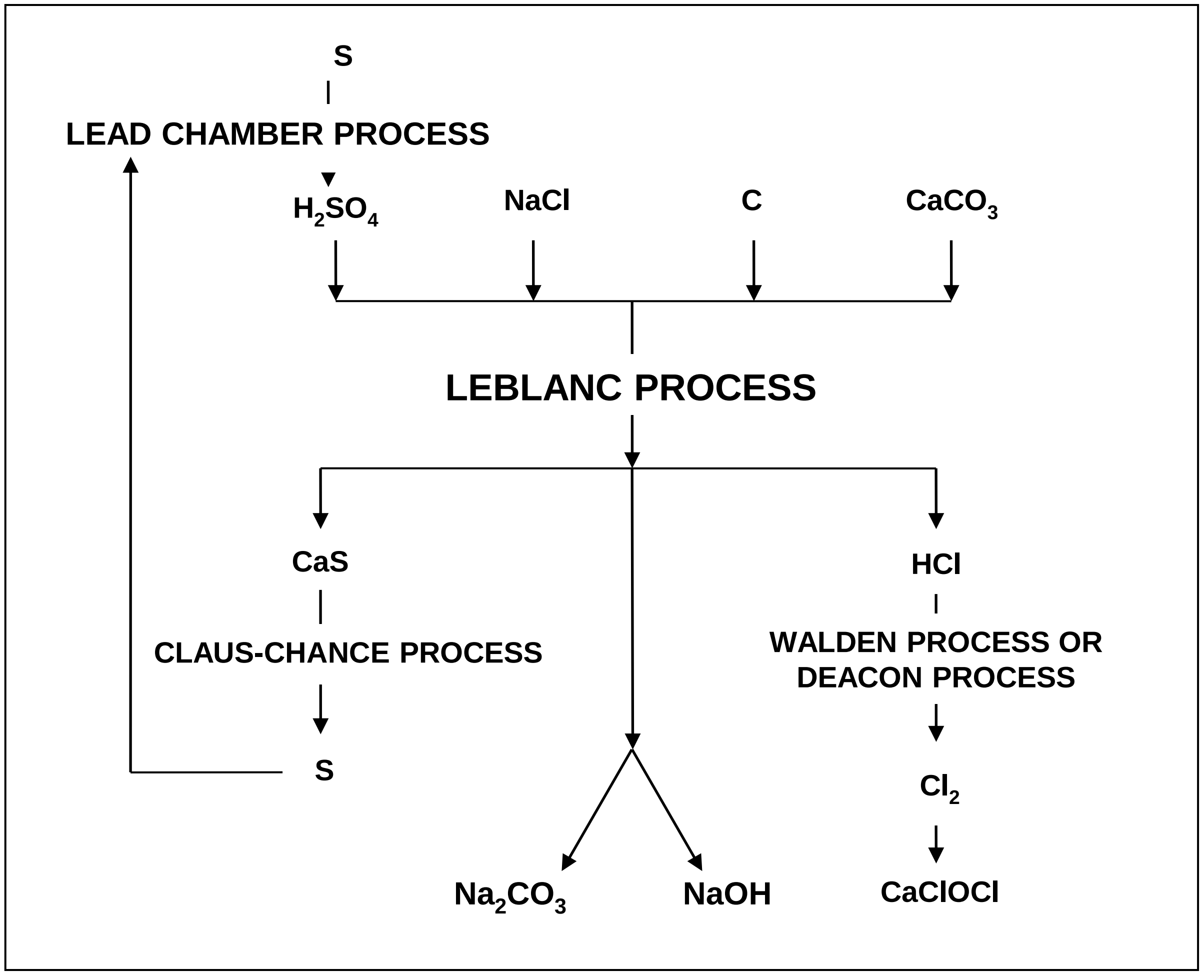
CENTERED AT THE LEBLANC PROCESS

EARLY EXAMPLE OF INDUSTRIAL ECOLOGY

IMPORTANCE FOR THE

INDUSTRIAL PRACTICE OF CHEMISTRY

EARLY GC" (25): LEBLANC ➔ SOLVAY



EARLY GC” (26): LEBLANC ➔ SOLVAY

E-FACTORS:

LEBLANC PROCESS VS ECO-INDUSTRIAL SYSTEM (UK)

LEBLANC PROCESS (1863): E-FACTOR = 5,3

280.000 TON OF SODA FROM 1.760.000 TONS OF RAW-MATERIALS

ECO-INDUSTRIAL SYSTEM (LATER, ?): E-FACTOR = 2

3.000 UNITS OF SALABLE PRODUCTS FROM 9.000 UNITS OF RAW-MATERIAL

CALCULATED THEORETICAL VALUE (ASSUMING S & Cl FULLY RECOVERED)

E-FACTOR = 1,98

GOOD EFFICIENCY OF ECO-INDUSTRIAL SYSTEM:

HIGH ATOM PRODUCTIVITY!

EARLY GC" (27): LEBLANC → SOLVAY

2

NON-TECHNICAL CAUSES SUPPORTED THE LEBLANC PROCESS

1

1891

UK COMPANIES (> 40) AGGLOMERATED → UNITED ALKALI CO

ONLY EFFICIENT PLANTS WERE KEPT

2

SITUATION OF PATENTS FAVORED THE UNITED ALKALI CO

AGREEMENT ABOUT PRICES/MARKET QUOTAS

WITH THE COMPETITOR (MOND)

EARLY GC" (28): LEBLANC ➔ SOLVAY

PENETRATION OF NEW GREENER PROCESSES

SLOWED DOWN BY ECONOMIC & OTHER REASONS

BEGINNING OF THE 20TH CENTURY

DEATH OF LEBLANC PROCESS

ELECTROLYTIC PROCESS: Cl_2 & NaOH

REVOLUTION OF THE ALKALI INDUSTRIAL SECTOR

(ELECTRICITY ≡ ENERGY)

EARLY GC" (29): LEBLANC → SOLVAY

RECENT DEVELOPMENT: US, 1986

LAST SOLVAY PLANT CLOSED DOWN

Na_2CO_3 OBTAINED FROM

- TRONA (MINERAL
- BRINES

ONLY RECRYSTALLIZATION : NO CHEMISTRY

SIMPLER

≈ 1/2 THE COST

EARLY GC" (30): LEBLANC ➔ SOLVAY

IN FAVORABLE CASES

NO CHEMISTRY IS GOOD GC

EARLY GC" (31): LEBLANC → SOLVAY

~~IN [illegible]RA[illegible] CASES~~

~~NO CHE[illegible]TR[illegible] GOOD GC~~

EARLY GC" (32): LEBLANC → SOLVAY

CONCLUSION

PROCESS REPLACEMENT: LEBLANC → SOLVAY

VERY RICH EXAMPLE FOR GC

- PROCESS SUBSTITUTION AIMED AT GREENNESS
- PREVENTION OF RESIDUES BY RECYCLING
- IMPORTANCE OF ECO-INDUSTRIAL SYSTEMS
- NON-CHEMISTRY BARRIERS THAT SLOW SUBSTITUTION

EARLY GC" (33): CONCLUSIONS

INDUSTRIAL SYSTEMS IN THE PAST:

WHEN STRONG NEGATIVE IMPACTS WERE FOUND CHEMISTS PROVIDED ALTERNATIVES TO MINIMIZE/ELIMINATE THE PROBLEMS

↓

GLOBAL PURPOSE OF GC AT PRESENT

NOT NEW FOR CHEMISTRY!!!

EARLY GC" (34): CONCLUSIONS

HISTORY OF "EARLY" GC

ELIMINATION OF NEGATIVE IMPACTS BY PEOPLE WHO

- BUILT AND MANAGED INDUSTRIAL SYSTEMS
- HAD ACQUIRED A SYSTEMS THINKING MINDSET

SUGGESTS THAT

SYSTEMS THINKING IS WORTH USING IN GC

EARLY GC" (35): CONCLUSIONS

INCISIVE ADVICE TO STUDENTS

EARLY CHEMISTS USED GC IN THE PAST WITHOUT KNOWING WHAT IT WAS…

… NOW THAT KNOW IT…

…IT WILL BE MUCH EASIER TO DEVELOP GC

AS A SYSTEMATIC PRACTICE

SYSTEMS THINKING & GC (1)

SYSTEMS THINKING PRESENTATION OF GC

PROVIDES

A GLOBAL UNIFIED VISION OF ITS ACTIVITIES

SHOWS

THE COMPLEXITY OF RE-SHAPING CHEMISTRY TO GC

SYSTEMS THINKING & GC (2)

SYSTEMS COMPONENTS

MATTER, ENERGY & INFORMATION

MUST BE CONSIDERED

- **TOGETHER**
- **INCLUDING THEIR INTERCONNECTIONS**

FOR HOLISTIC MANAGEMENT OF THE SYSTEM

➔OBJECTIVE

SYSTEMS THINKING AND GC (3)

SYSTEMS APPROACH TO GC

MEANS

- JOINT OPTIMIZATION OF THE 3 COMPONENTS
- SIMULTANEOUS INCREASE OF THEIR **PRODUCTIVITIES**

SYSTEMS THINKING & GC (4)

PRODUCTIVITY

(ECONOMICS)

AMOUNT OF PRODUCT PER UNIT OF PRODUCTION FACTOR USED

PRODUCT IMBUED WITH GREENNESS

SYSTEMS THINKING & GC (5)

"SYSTEMIC CHEMISTRY": GC OBJECTIVES

USE OF LESS …

1 - MATTER: ***DEMATERIALIZATION***

2 - ENERGY: ***"DENERGIZATION"***

≡ ↓ ENERGY INTENSITY

3 - INFORMATION: ***"DEINFORMATION"***

≡ SIMPLIFICATION

SYSTEMS THINKING & GC (6)

SIMPLIFICATION:

MANAGEMENT OF

SIMPLER SYSTEMS

REQUIRES

LESS INFORMATION

(INVOLVES LESS KNOWLEDGE)

SYSTEMS THINKING & GC (7)

GC HAS BEEN PURSUING

THESE OBJECTIVES

SINCE ITS EMERGENCE

SYSTEMS THINKING & GC (8)

DEMATERIALIZATION

- SYNTHETIC PATHWAYS WITH LARGE ATOM ECONOMY
- CATALYTIC INSTEAD OF STOICHIOMETRIC REACTIONS
- ELIMINATION OF GROUP PROTECTION
- SEPARATION & RECYCLING OF REAGENTS
- ...

SYSTEMS THINKING & GC (9)

ENERGY INTENSITY REDUCTION

- CATALYSTS: ↓ REACTION TEMPERATURE
- ALTERNATIVE TECHNOLOGIES FOR PROVIDING ENERGY TO THE REACTOR:

↓ CONSUME VS. HEATING

…

SYSTEMS THINKING & GC (10)

SIMPLIFICATION

TWO TYPES OF MEASURES

ADRESSED TO…

1 - THE EXTERNAL IMPACTS

2 - THE CHEMISTRY

SYSTEMS THINKING & GC (11)

SIMPLIFICATION OF IMPACTS

- ELIMINATION OF TOXIC PRODUCTS
- NO USE OF DANGEROUS/TOXICS SUBSTANCES IN SYNTHESIS
- …

SYSTEMS THINKING & GC (12)

VERY BROAD SCOPE : LESS IMPACTS ≡ …

ENVIRONMENT:

… ≡ MORE PROTECTION

ECONOMY:

… ≡ LESS LEGISLATION & CONTROL ≡ LESS COSTS

SOCIETY:

… ≡ BETTER HEALTH & QUALITY OF LIFE

SYSTEMS THINKING & GC (13)

SIMPLIFICATION OF CHEMISTRY

- SYNTHETIC PATHWAYS WITH LESS STEPS
- TELESCOPING STEPS ALONG PATHWAYS
- ELIMINATION OF REACTION SOLVENT
- RATIONALIZATION OF SOLVENTS
- ...

SYSTEMS THINKING & GC (14)

SIMPLIFICATION OF CHEMISTRY

IMPORTANT …

… TO DECREASE THE REQUIREMENTS OF CHEMICAL INFORMATION

BUT ALSO…TO FACILITATE

DEMATERIALIZATION AND "DENERGIZATION"

SYSTEMS THINKING & GC (15)

CROSSED INTERACTIONS

BETWEEN

MATTER, ENERGY & INFORMATION

LINEAR DESCRIPTION:

SIMPLISTIC

SYSTEMS THINKING & GC (16)

CROSSED INTERACTIONS - WIDESPREAD!

SEPARATION & RECYCLING

CONTRIBUTES TO DEMATERIALIZATION (↑)
BUT … REQUIRES ENERGY (↓)

DEMAT… AND "DENERG…" CONFLICT:
OPTIMIZATION REQUIRED TO FIND A BALANCE

DIFFERENT FROM CASE TO CASE:
IF SEPARATION REQUIRES A HUGE AMOUNT OF ENERGY
RECYCLING DOES NOT PROVIDE GREENNESS

SYSTEMS THINKING & GC (17)

SIDE REMARK

IMPORTANCE OF ENERGY IN CHEMISTRY

SCARCE ATTENTION PAID TO ENERGY

IN THE TEACHING LABORATORIES OF SYNTHESES

MATTER-ENERGY INTERACTION REQUIRES

MORE ATTENTION!

SYSTEMS THINKING & GC (18)

MATTER, ENERGY & INFORMATION

LINEAR MODEL :

ASSUMES THE ORTHOGONALITY OF PRODUCTIVITIES

NOT VALID IN MOST SITUATIONS:

CROSSED INTERACTIONS!

SYSTEMS THINKING & GC (19)

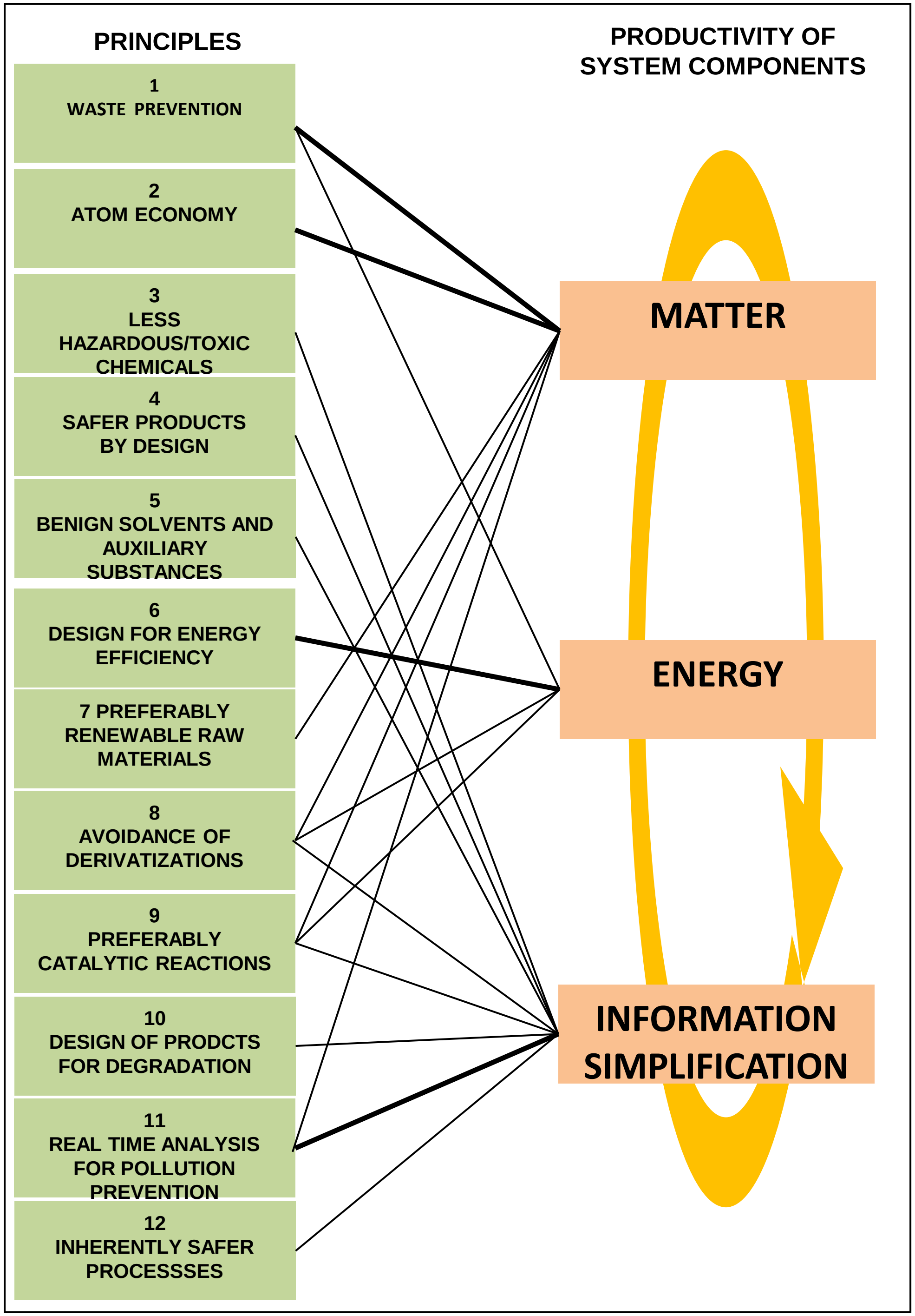
GREENNESS

INVOLVES…

- A LARGE NUMBER OF FACTORS
- A LARGER NUMBER OF INTERCONNECTIONS

VERY COMPLEX CONCEPT

FIG. 4



INTERACTIONS: NUMEROUS COMPLEX

SYSTEMS THINKING & GC (21)

FACTORS & INTERACTIONS

CHANGE

ALONG THE WAY

LABORATORY → FINAL USE OF CHEMICALS

GREENNESS CHAIN

OF CHEMISTRY

SYSTEMS THINKING & GC (22)

THE GREENNESS CHAIN

GREEN (LABORATORY) CHEMISTRY

GREEN SYNTHESIS

GREEN SCALE-UP

GREEN CHEMICAL ENGINEERING

GREEN PROCESS DEVELOPMENT

GREEN CHEMICAL INDUSTRY

GREEN MANUFACTURING

GREEN FORMULATION

GREEN (SOCIETY) USE

GREEN USE OF CHEMICALS

SUSTAINABLE DEVELOPMENT

SYSTEMS THINKING & GC (23)

GREENNESS ITSELF

MUST BE EVALUATED UNDER A

LIFE-CYCLE PERSPECTIVE

FOR IDEAL PURPOSE OF MAXIMIZING IT CUMULATIVELY UP TO THE END OF CHAIN

SYSTEMS THINKING & GC (24)

IMPORTANCE OF G (LABORATORY) C

WITHOUT GREENNESS AT DEPARTURE

IMPOSSIBLE

GREENNESS AT THE END OF CHAIN

SYSTEMS THINKING & GC (25)

NATURE OF THE GREENNESS IMBUED IN THE PRODUCT & SYNTHETIC PATHWAY

GREENNESS IN THE LABORATORY

MUST BE SUITABLE

TO BE KEPT ALONG THE CHAIN

SYSTEMS THINKING & GC (26)

SYSTEMS THINKING APPROACH TO GC

1

SHOWS

- ITS COMPLEX NATURE
- DIFFICULTIES OF IMPLEMENTATION
- ADVANTAGES OF EQUIPING CHEMISTRY STUDENTS MIND WITH A SYSTEMIC COMPONENT

SYSTEMS THINKING & GC (27)

2

ASKS FOR MORE ATTENTION TO

- INTERACTIONS AMONG THE VARIABLES OF GC
- IMPORTANCE OF MULTI-DIMENSIONAL CHOICES
- NEED OF TOOLS FOR MULTI-CRITERIA DECISIONS
- …

HOLISTIC GC METRICS (1)

COMPLEXITY OF GREENNESS

↓

ASSESSMENT IS DIFFICULT

↓

DIFFERENT METRICS USED ALONG THE GREENNESS CHAIN

- SEVERAL TYPES
- IN VARIOUS CONTEXTS

HOLISTIC GC METRICS (2)

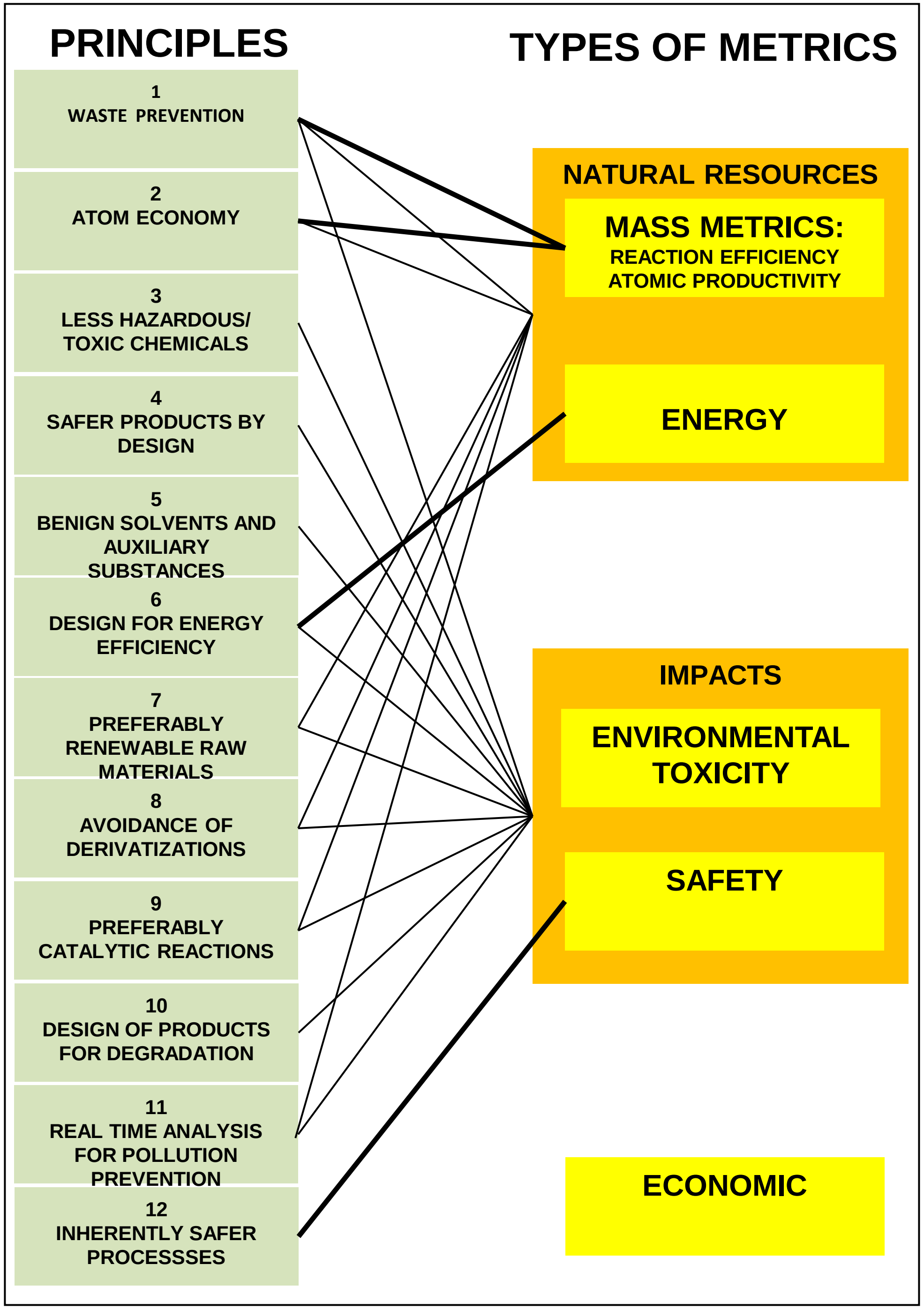
GC TEACHING IN THE LABORATORY:

METRICS TO BE USED BY STUDENTS?

12 PRINCIPLES ≡ DESIRABLE INFRASTRUCTURE FOR SELECTION OF METRICS FROM LITERATURE

COMPLEX NET OF CONNECTIONS

FIG. 6



FOR IMPACT METRICS: INTERACTIONS: ARE COMPLEX

HOLISTIC GC METRICS (4)

SIMPLE & INTUITIVE MASS METRICS

E-FACTOR/ATOM ECONOMY/MASS INTENSITY

↓

SUITABLE FOR EVALUATION OF CHEMISTRY:

REACTION EFFICIENCY & ATOM PRODUCTIVITY

METRICS FOR ENVIRONMENTAL & TOXICITY IMPACTS:

TOO COMPLEX FOR USE IN LAB

HOLISTIC GC METRICS (5)

SYSTEMS THINKING

↓

HOLISTIC METRICS

CAPTURE OF A LARGE NUMBER OF GREENNESS FEATURES

↓

DESIGN OF SIMPLE SEMI-QUANTITATIVE METRICS

BASED ON THE 12 PRINCIPLES

HOLISTIC GC METRICS (6)

GREENSTAR (GS)

1

EACH OF THE 12 PRINCIPLES: EVALUATION OF ACCOMPLISHMENT
(STANDARDIZED PROCEDURES - SCORE 1 TO 3)

2

SCORES REPRESENTED IN A RADAR CHART (STAR)
NUMBER OF CORNERS = NUMBER OF PRINCIPLES ASSESSED

3

SIMPLE VISUAL INSPECTION:
AREA OF THE STAR ≡ SEMI-QUANTITATIVE VIEW OF THE GREENNESS

THE LARGER THE AREA, THE GREENER IS THE REACTION

HOLISTIC GC METRICS (7)

CHANGE OF EXPERIMENTAL REACTION CONDITIONS

↓

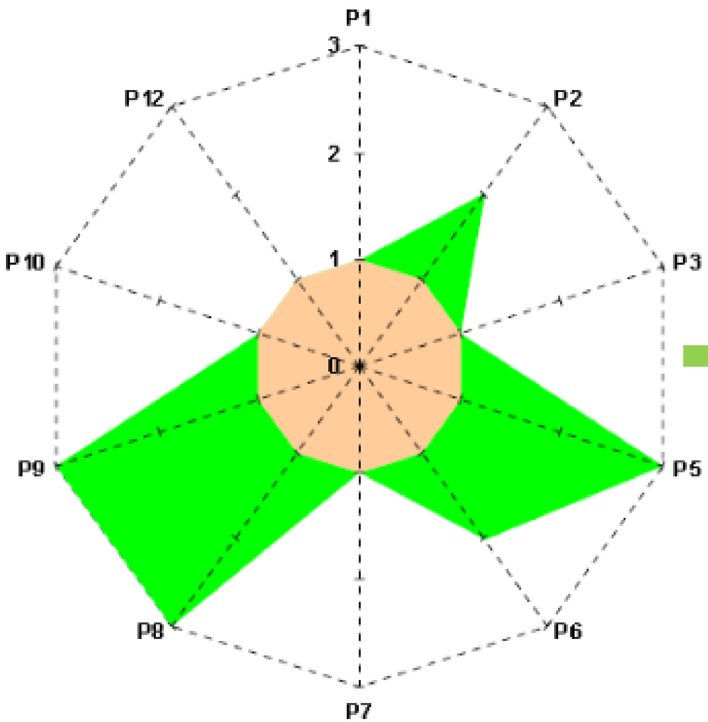
GS CAPTURES EFFECTS ON EACH PRINCIPLE

COMPARISON OF GS´S BEFORE/ AFTER :

- **PROGRESS IN GREENNESS**
- **IDENTIFICATION OF THE WORSE ITEMS FOR FURTHER IMPROVEMENT**

HOLISTIC GC METRICS (8)

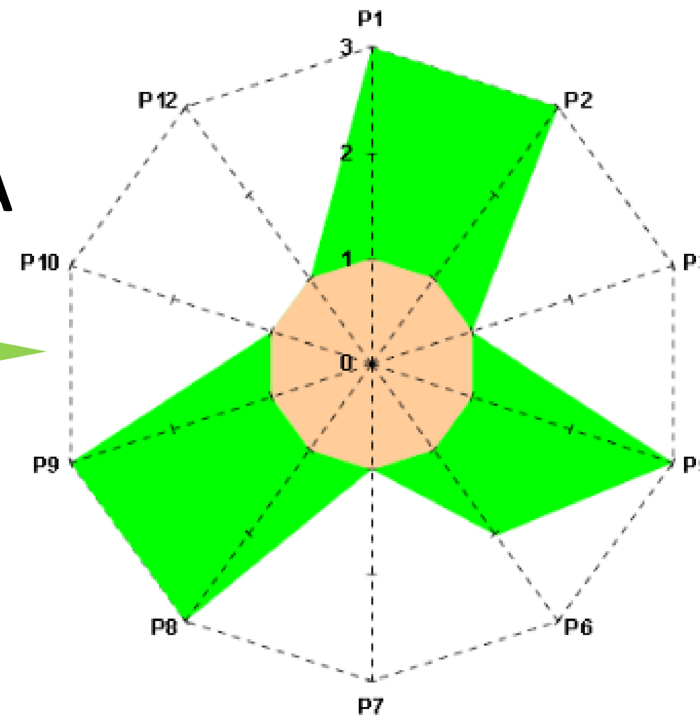
TETRAMMINE-COPPER(II) SULFATE MONOHYDRATE



LESS EXCESS OF AMMONIA

300% → 7%

INCREASE OF GREENNESS



HOLISTIC GC METRICS (9)

OTHER 2 HOLISTIC METRICS

UNDER EVALUATION

- GREEN MATRIX (SWOT ANALYSIS)
- GREEN CIRCLE

HOLISTIC GC METRICS (10)

GS USED EXTENSIVELY BY STUDENTS IN

A GC LABORATORY TEACHING PROCEDURE:

MORE ACTIVE PARTICIPATION IN

- PURSUING GREENNESS
- LEARNING THE PURPOSE & PRACTICE OF GC

STRATEGY TO GC TEACHING IN LAB (1)

CHALLENGE TO THE STUDENTS:

TO IMPROVE

SYNTHESIS PROTOCOLS

IN TEXTBOOKS TO

INCREASE GREENNESS

STRATEGY TO GC TEACHING IN LAB (2)

1

ASSIGNMENT OF A COMPOUND/PROTOCOL

2

SYNTHESIS IN THE LABORATORY & GREENNESS EVALUATION

(MASS METRICS + GS)

3

ANALYSIS OF THE PROTOCOL FOR IMPROVEMENT BY CHANGING CONDITIONS

TEMPERATURE/EXCESS OF REAGENTS/SOLVENTS, ETC.

4

NEW SYNTHESIS IN THE LABORATORY &

ASSESSMENT OF THE GREENNESS IMPROVEMENT

STRATEGY TO GC TEACHING IN LAB (3)

5

REPETITION OF THE TASK:

CORRECTION OF BAD CHOICES OF CONDITIONS

OR

FURTHER INCREMENT OF GREENNESS

STRATEGY TO GC TEACHING IN LAB (4)

RESULTS

VERY SIMPLE INORGANIC SYNTHESIS

TABLE 6

TABLE 6 RESULTS OF THE OPTIMIZATION OF PROTOCOLS OF SYNTHESES

COMPOUND	LIGAND/METAL	IMPROVEMENT OF THE GREENNESS (GS, % OF MAXIMUM GREENNESS)
	AMMONIA	
$[Cu(NH_3)_4](SO_4).\ H_2O$		27,5 → 40,00
	OXALATE	
$Fe(II)OX_3.2\ H_2O$		20,00 → 36,25→ 41,25 → 46,25
	ACETYLACETONATES	
$FE(III)ACAC_3$		32,50 → 40,0
		41,25 → 51,25
		30,0
$M(II)ACAC_2$	Mn OR Mg	22,50 → 30,0
	Ca	46,25 → 57,50

STRATEGY TO GC TEACHING IN LAB (6)

MOST PROTOCOLS PRESCRIBE

LARGE EXCESS OF A REAGENT

WHICH IS NOT NECESSARY!

STRATEGY TO GC TEACHING IN LAB (7)

ADVANTAGES

- REQUIRES CREATIVE THINKING ALONG PARALLEL LINES TO DEVISE IMPROVEMENTS
- DEVELOPS THE CAPACITY FOR MAKING CHOICES/ASSUMING THE RESPONSIBILITY OF TAKING DECISIONS
- STRESSES THAT GC REQUIRES A SYSTEMS THINKING STRATEGY

STRATEGY TO GC TEACHING IN LAB (8)

MAIN LIMITATION

STUDENTS REQUIRE A LOT OF

SUPPORT/SUPERVISION

IN THE LABORATORY

↓

LIMITED NUMBER OF STUDENTS (<6)

CONCLUSIONS (1)

CHEMISTRY IS INTRINSICALLY COMPLEX

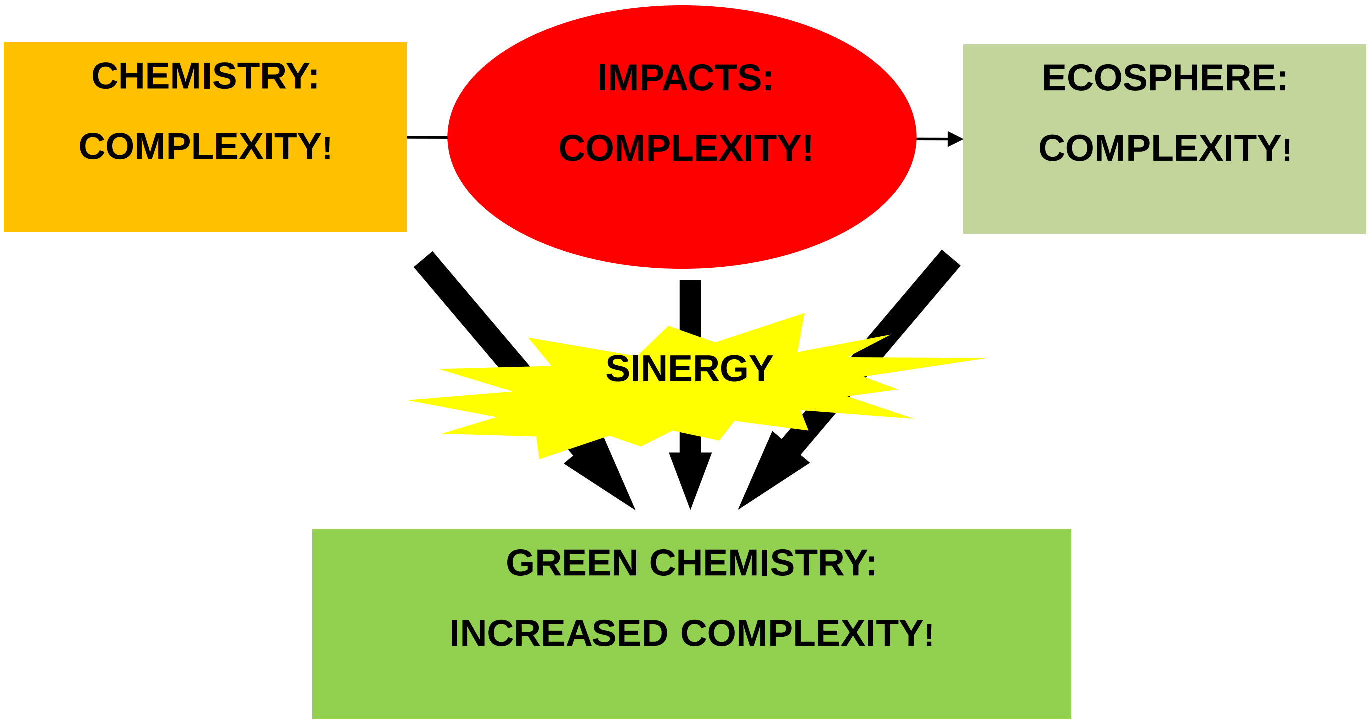
GREENNESS IS STILL MORE COMPLEX

↓

COMPLEXITY IS FURTHER INCREASED WHEN GREENNESS IS AIMED IN GREEN CHEMISTRY

CONCLUSIONS (2)

SINERGY IN THE COMPLEXITY OF GREEN CHEMISTRY



CONCLUSIONS (3)

GC INVOLVES AN

EXTREMELY COMPLEX NET OF INTERACTIONS

SIMPLE CAUSE-EFFECT RELATIONSHIPS

(CARTESIAN REDUCTIONISM)

PROVIDE NO GOOD DESCRIPTION OF SITUATIONS WITH LARGER NUMBERS OF INTERCONNECTIONS

CONCLUSIONS (4)

HOLISTIC MINDSET: SYSTEMS THINKING TO DEAL WITH INTERCONNECTIONS TO…

- ANALYZE THEIR RELATIVE STRENGTH & IMPORTANCE IN EACH SITUATION
- ELIMINATE THE DANGEROUS CONNECTIONS
- BALANCE CONFLICTING OUTCOMES
- …

CONCLUSIONS (5)

- IMPORTANT TO DEVELOP

  THE SYSTEMS THINKING

  CAPACITIES OF CHEMISTRY STUDENTS

  - NOT AN EASY TASK

- THIS WORK: ONLY A VERY PRELIMINARY EFFORT!

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