Recipes for Data Rectification of Life Cycle Inventories

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Life cycle inventory

contents	unit	amount	contents	unit	amount
Coal	lb	68.1	BOD	lb	1.9E-05
Electricity	kWh	813.0	Chlorine	lb	3.2E-04
Natural gas	lb	202.0	Dissolved Solids	lb	4.3
Residual oil	gallons	3.8	Lead	lb	9.4E-07
salt	lb	1670.0	Mercury	lb	5.4E-04
			Mercury	lb	1.5E-06
			Nickel	lb	9.4E-07
			Particulates	lb	4.6E-04
			Solid waste	lb	3.1E+00
			Sulfides	lb	1.5E-04
			Sulfur oxides	lb	1.0E-03
			Zinc	lb	9.4E-07
			Chlorine/Caustic Soda Production	lb	1000.0
			Chlorine	lb	893.0
			Hydrogen	lb	16.9
Total		1943.9			1917.3

(NREL NaOH LCI)

Data inconsistency

- **Commensurability**
  - BOD cannot be added directly to output material
  - In certain LCI, energy consumption is represented by kJ, kWh, etc.
- **Discrepancy**
  - Conservative law of mass is not satisfied
- **Aggregated chemical species**
  - Dissolved solids, particulate and sulfides contains several chemical components

Possible problems from inconsistency

- **Data discrepancy**
  - **Missing flows** in resource consumptions and waste emissions make impact analysis of chemical species ignored.
  - LCA results may be not correct from the **incorrect measured values**
  - Decision making by LCA is not correct if using discrepant LCI.
  - Data rectification can be applied to deal with the data discrepancy

- **Incommensurability and Aggregated species**
  - make data rectification difficult or practically impossible

Data rectification of LCI and process engineering

	LCI	Process engineering
Redundancy	Nonredundant	A few redundancy
Infrastructure	Blackbox	Detail flowsheets
Time horizon	One point	Yearly, monthly, daily, hourly, etc.
Aggregated species	Particulate, NOx, SOx, etc.	None
Reaction model for (trace) waste	Important	Not so important
Included process	Several processes	One process
Data source	Multiscale	One scale

Objectives

- **Propose methodology to deal with data discrepancy of LCI**
  - Multiscale characteristics of LCI data is used for rectification
  - Reducing procedure of the large number of models due to several included processes is shown
  - Nonredundancy of LCI data is solved by atomic balance

Data rectification in process engineering

- **Gross error detection and identification**
  - Global test: $\gamma = \mathbf{r}^{\mathrm{T}} \mathbf{V}^{-1} \mathbf{r} \sim \chi_v^2$
  - Nodal test $z_{r,i} = r_i / \sqrt{V_{ii}} \sim N_i(0,1)$
  - Measurement test $z_{d,j} = \left| y_j - x_j \right| / \sqrt{W_{jj}} \sim N(0,1)$

- **Data reconciliation**

$$\min_{\mathbf{x}} \quad f = \boldsymbol{\varepsilon}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\varepsilon}$$

$$s.t.$$

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$$

$$\text{where} \quad \mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon}$$

Data rectification in process engineering

- **Simultaneous gross error compensation and reconciliation**

$$\min_{\mathbf{x},\boldsymbol{\delta},\mathbf{B}} \quad f = \boldsymbol{\varepsilon}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\varepsilon}$$

$$s.t.$$

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

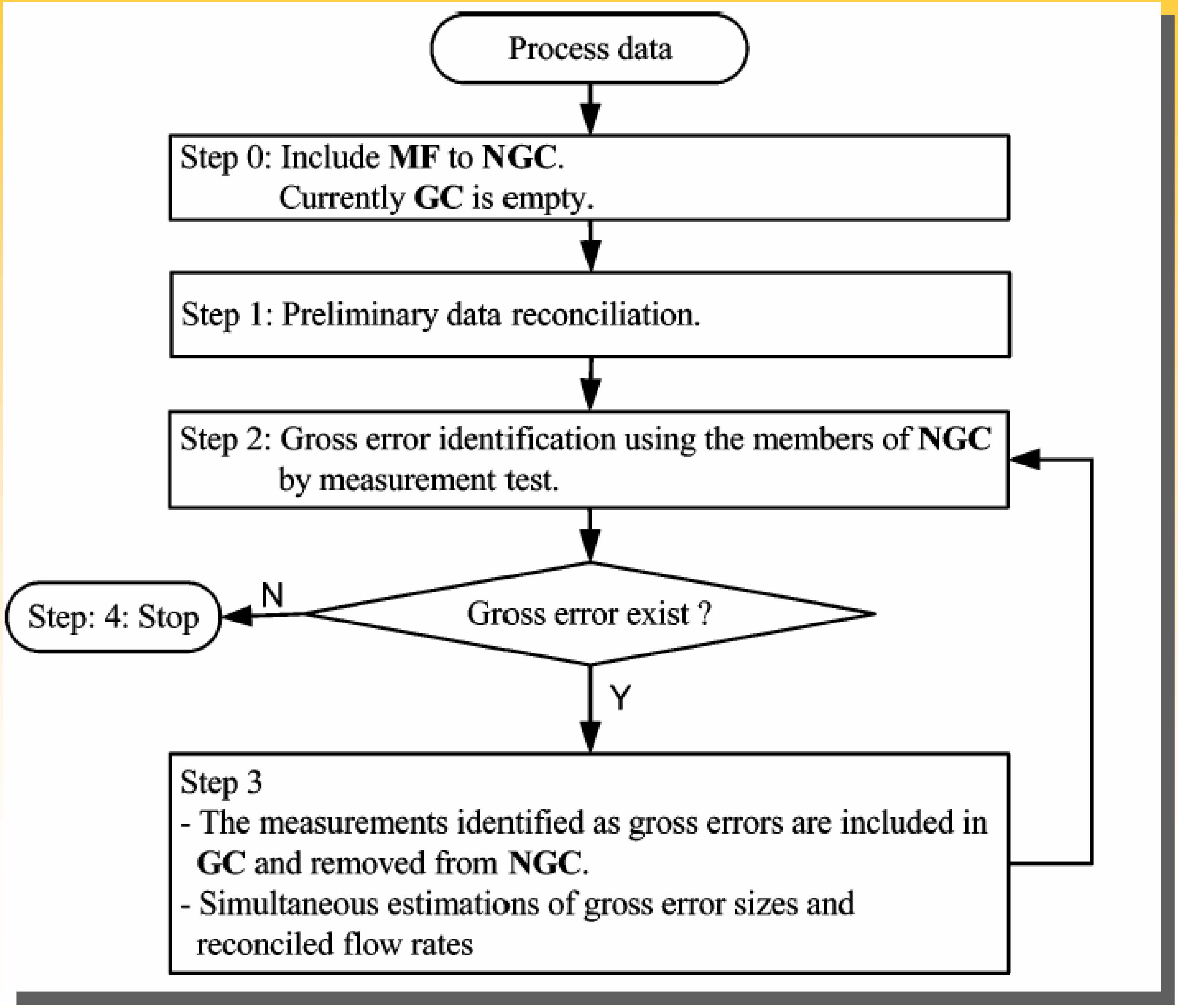
$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$$

$$|\delta_i| - U_i B_i \leq 0$$

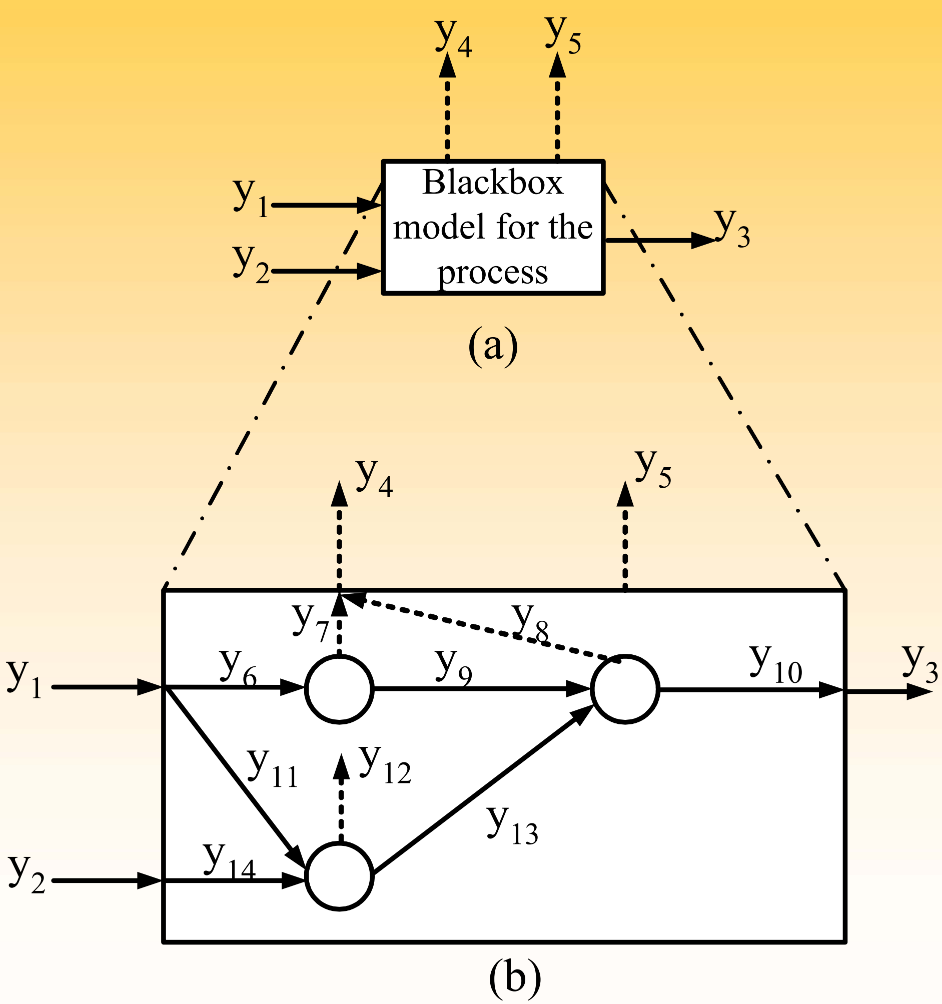
$$|\delta_i| - \zeta_i U_i B_i \geq 0$$

$$\text{where} \quad \mathbf{y} = \begin{cases} \mathbf{x} + \boldsymbol{\varepsilon} + \boldsymbol{\delta} & \text{for the variable that gross error is identified} \\ \mathbf{x} + \boldsymbol{\varepsilon} & \text{for the others} \end{cases}$$

Data rectification in process engineering



LCI data rectification – multiple scales



Objective functions

- Type I. Commonly exist at both scales

  e.g., (y2, y14), (y3, y10)

$$u_2 \frac{(y_2 - x_2)^2}{\sigma_2^2} + u_{14} \frac{(y_{14} - x_{14})^2}{\sigma_{14}^2}$$

where $u_2 + u_{14} = 1$

- Type II. Aggregated at coarse scale

  e.g., (y4, y7, y8), (y1, y6, y11)

$$u_4 \frac{(y_4 - x_7 - x_8)^2}{\sigma_4^2} + u_7 \frac{(y_7 - x_7)^2}{\sigma_7^2} + u_8 \frac{(y_8 - x_8)^2}{\sigma_8^2}$$

where $u_4 + u_7 + u_8 = 1$

- Type III. Exist only at fine scale

  e.g., y9, y12, y13

- Type IV. Exist only at coarse scale

  e.g., y5

LCI data rectification – confining models

- **LCI data**
  - Several processes are included for LCI data
  - It is required to confine models for problem size reduction
- **Process models**
  - Generally, the balance equations of total mass and component are used
  - Component balances are not required for the node that does not have gross errors

i) Implement global test by total mass balances

ii) If (no error is detected) then
    go to step vii)
  else
    continue

iii) Implement nodal test for each node by total mass balances

iv) Add component balances in the descending order of nodal test statistics values

v) Calculate the global test statistics

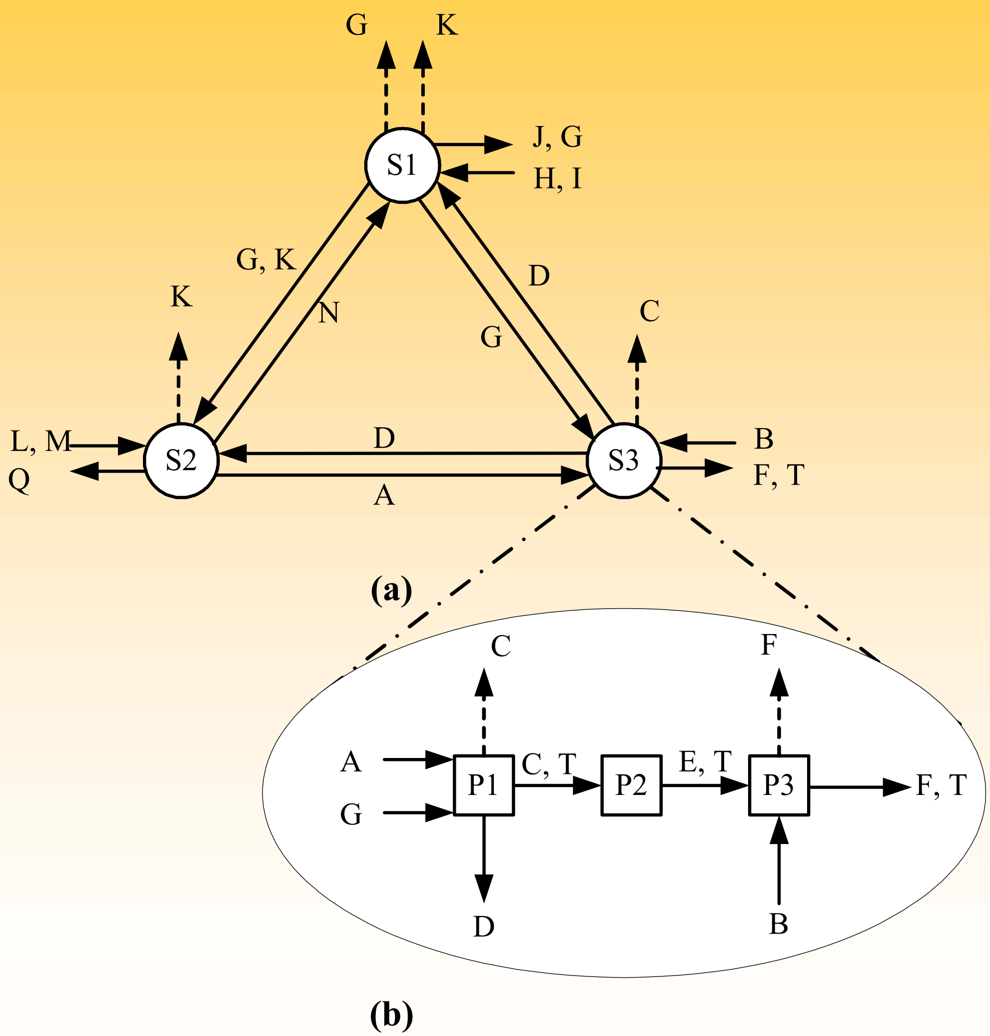
vi) if (Δglobal test statistics) > (predefined criterion) then
    go to step iv)
  else
    continue

vii) Preliminary data reconciliation

viii) Measurement test for gross error identification

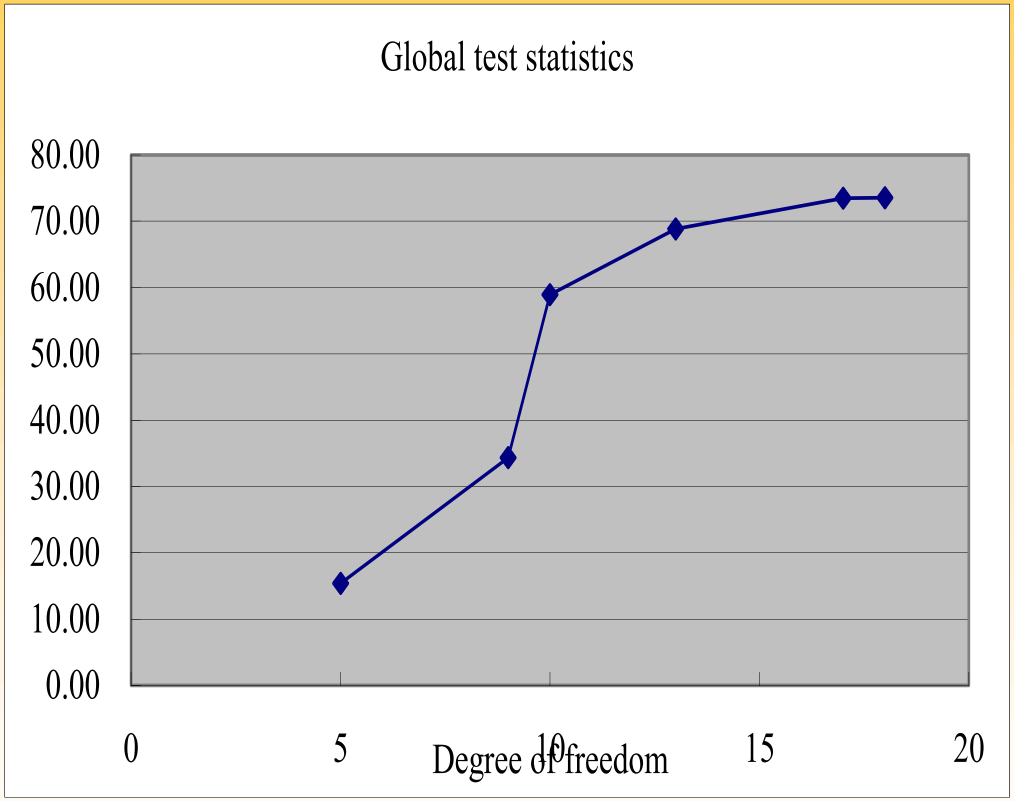
ix) Simultaneous gross error compensation

LCI data rectification – confining models



- **The number of constraints**
  - 18 equations are required for complete component balances
- **The number of equations can be reduce by applying the proposed procedure**
- **The rectification results by the proposed algorithm are not changed significantly compared with complete constraints**

LCI data rectification – confining models



- The sums of relative errors for highest three cases are shown for comparison

	DOF=13	DOF=17	DOF=18
Sum of Rel. err	0.19	0.16	0.12

LCI data rectification – nonredundancy

- **Public LCI data often neglect certain chemicals**

Component	Mass, kg	
	Input	Output
Natural gas (fe	464.0	
H2O	922.0	
CH4		7.14
CO		2.50E-02
CO2(emission)		4.36E-01
NMVOC		9.28E-01
NO2		3.04E-01
SO2		1.00E-02
CO2(co-product)		1155.9
NH3		1000.0
Total	1386.0	2157.6

(SimaPro NH3 LCI)

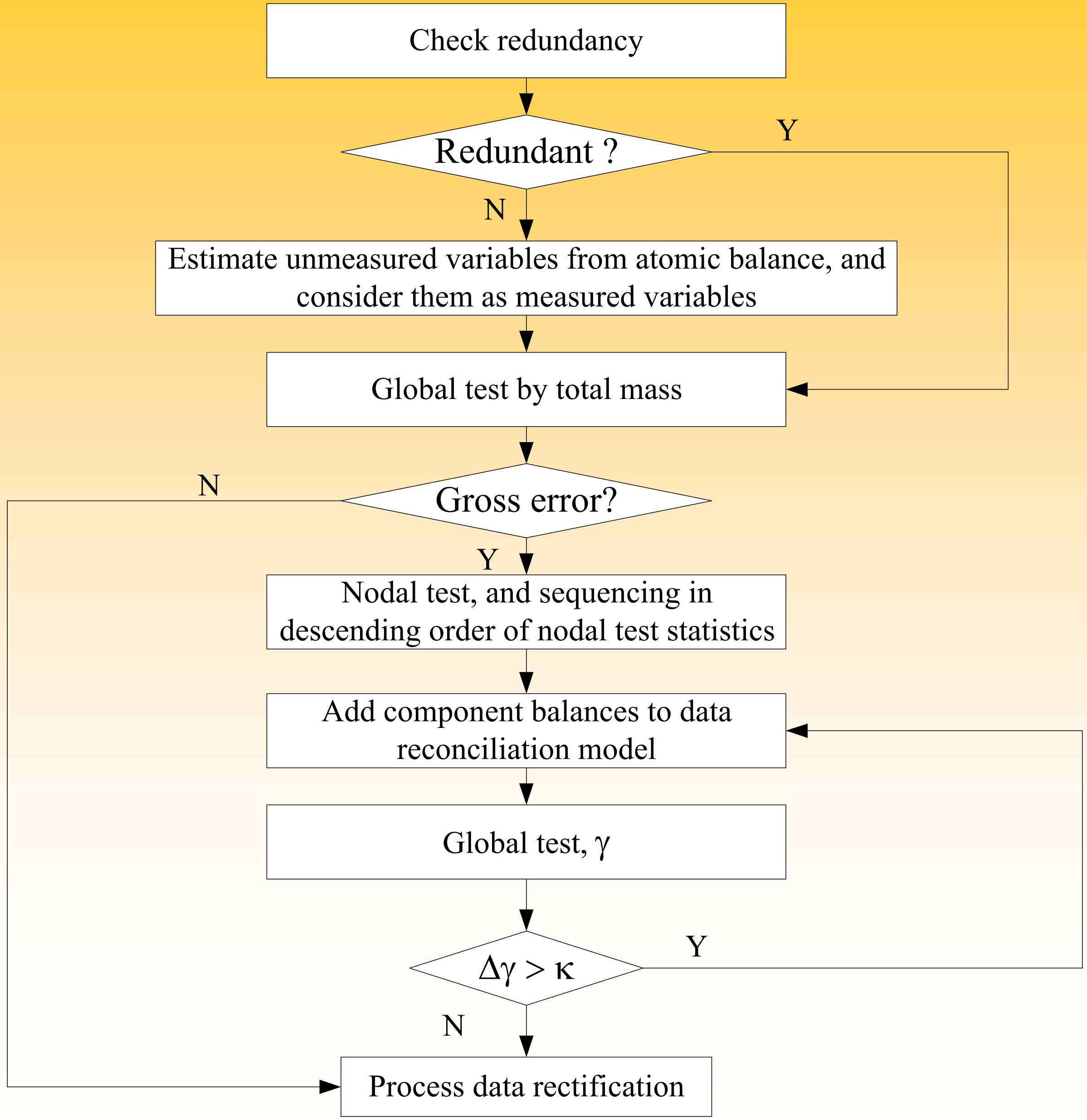
- **Ammonia process consumes H2O and O2 for resources**

- **O2 and H2O are estimated by atomic balance**

Component	Mass, kg	
	Input	Output
Natural gas	464.0	
H2O	922.0	
O2	17.8	
N2	822.4	
CH4		7.14
CO		2.50E-02
CO2(emission)		4.36E-01
NMVOC		9.28E-01
NO2		3.04E-01
SO2		1.00E-02
CO2(co-product)		1155.9
NH3		1000.0
Total	2226.3	2157.6

- **Only if the estimated O2 and H2O are considered as measured variables, the system is redundant**

Algorithm for LCI data rectification



Future work and conclusion

- **The methodology for LCI data rectification is proposed**
  - Multiscale data could be cooperated for data rectification
  - Large size of constraints could be reduce by confining procedure of process models
  - Nonredundancy problem is deal with atomic balance, which make system redundant

- **The proposed methodology will be applied to life cycles of LNG power plant and ammonium nitrate plant**