On the Quality of Waste Biomass Serving as a Substitute for Activated Carbon in Packed Bed Adsorption Columns

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Abstract: - This work deals with the quality improvement of modified waste biomass serving as a low-cost substitute for activated carbon in packed bed adsorption columns. Since the biomass modification cost depends on the partially conflict variables of operating and capital cost, we determined initially the optimal value of an Intensification Index as regards biomass thermochemical conversion; subsequently, we designed/developed a methodological framework under the form of an algorithmic procedure (including 21 activity stages and 8 decision nodes) in order to combine knowledge from Thermodynamics and Kinetics to find out the solution of the direct problem of determining the product quality according to production conditions. Finally, we solved the inverse problem of determining the conditions for either producing an adsorbent when specifications are given or improving its quality when the corresponding fault (set as top event in a Fault Tree Analysis structure) has been analyzed. An implementation example was used to prove the functionality/operability of our methodology when the top event is low rate of adsorption and the fault tree relations are given as fuzzy rules.

Key-Words: - waste biomass, quality, adsorption, packed bed columns, Fault Tree Analysis (FTA), fuzzy rules

1 Introductory Analysis

Waste biomass coming from agricultural/industrial residues (e.g., straw, cobs, husk, pomace, sawdust), unprocessed or processed thermochemically with salts, acids, alkalis, or solvents, can be used as a substitute for activated carbon in packed bed adsorption columns [1-3]. Since both adsorbents, thermochemically processed biomass and activated carbon, can be produced by the same lignocellulosic raw materials, the total production cost in combination with the adsorptive properties of the final product constitute the criteria for the decision making on optimal selection between them.

The total production cost C of thermochemically modified biomass is actually the sum of the partial costs C_1 and C_2, which represent operating (mainly due to energy consumption) and capital cost, respectively. Total cost minimization can be achieved by determining optimal values of the independent variables represented herein by an Intensification Index I. The partial cost C_1 is an increasing function of I with increasing rate (i.e., $dC_1/dI>0$, $d^2C_1/dI^2>0$), because of the Law of Diminishing Returns. The partial cost C_2 is a decreasing function of I with increasing algebraic or decreasing absolute rate (i.e., $dC_2/dI<0$, $d^2C_2/dI^2>0$ or $d|dC_2/dI|/dI<0$). I_{opt} is determined at $C_{min}= (C_1 + C_2)_{min}$ or $dC/dI=0$ or $d(C_1+C_2)/dI=0$ or $MC_1=MC_2$, where $MC_1=dC_1/dI$ and $MC_2=|dC_2/dI|$ are the marginal values of C_1 and C_2, respectively.

A decrease of energy cost, due either (i) to subsidy of operating (and/or waste biomass transportation) cost or (ii) to energy market price decrease, will move the $C_1(I)$ curve downwards to $C'_1(I)$, decreasing also MC_1, thus resulting to shift of I_{opt} to its new position I'_{opt} where $I'_{opt}>I_{opt}$ (Fig. 1a). If the subsidy is on the investment, thus decreasing the capital cost C_2, the corresponding $C_2(I)$ curve will move downwards to $C'_2(I)$, becoming also more flat, shifting I_{opt} to the new position I''_{opt}, where $I''_{opt}<I_{opt}$ (Fig. 1b).

The problem we deal with is how to combine (i) scientific expressed/explicit knowledge from Thermodynamics/Kinetics and (ii) empirical tacit/implicit knowledge obtained by means of human experts (either directly through questionnaires or indirectly through inference engines operating within an ‘expert system’ environment) in order to improve quality of waste biomass properly modified in accordance with the Best Available Technique Not Entailing Excessive Cost (known as BATNEEC in Environmental Management). This improvement should be the outcome of a flexible algorithmic procedure, designed/developed in a way that might facilitate implementation to various thermochemical processes using different lignocellulosic materials.

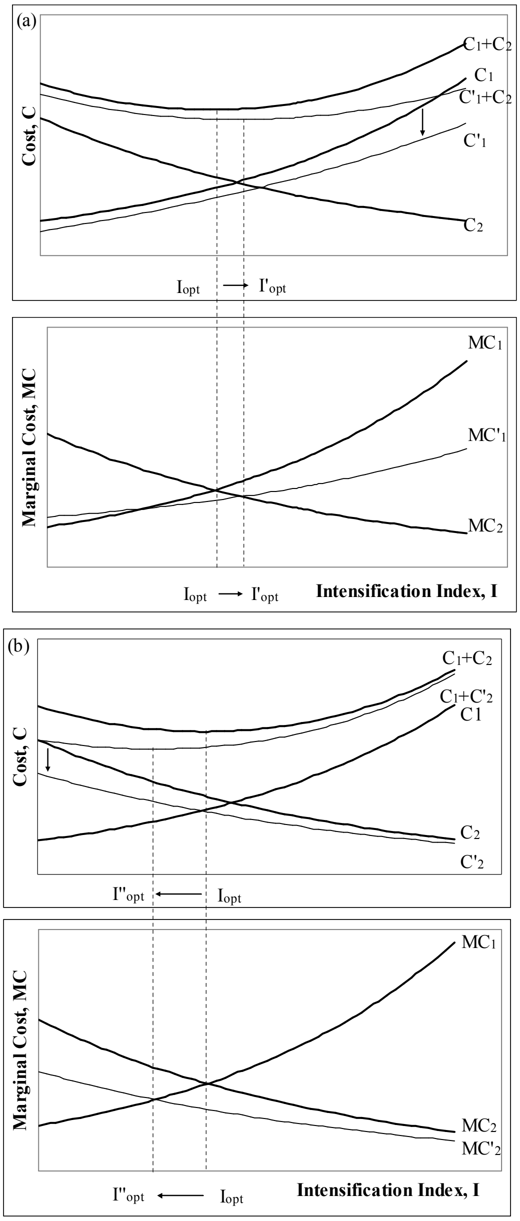

Fig. 1. Determination of I_{opt} at C_{min}, as described in the text: (a) the influence on I_{opt} of (i) subsidizing operating (including waste biomass collection/ transportation) cost or (ii) energy market price decrease, and (b) the influence on I_{opt} of subsidizing initial investment (implying capital cost decrease).

2 Methodology

The methodological framework, under the form of an algorithmic procedure based on Fault Tree Analysis (FTA), we have designed/developed for determining enhanced quality of waste biomass modified to serve as a low cost substitute for activated carbon in packed bed adsorption columns, is described below; the interconnection of stages/nodes is shown in Fig. 2.

1. Collection of data on modified biomass already in use as a low cost adsorbent.
2. Experimental design.
3. Performance of measurements.
4. Selection of isotherms to estimate adsorptive capacity.
5. Choice of the isotherm best fitted to data.
6. Synthesis/derivation of a new isotherm.
7. Experimental design for confirming the validity of the new isotherm using new significance level.
8. Fitting to experimental results.
9. Selection of kinetic models to estimate the rate of adsorption as a function of residence time.
10. Choice of the kinetic model best fitted to data.
11. Synthesis/derivation of a new kinetic model.
12. Experimental design for confirming the validity of the new kinetic model by using new significance level.
13. Fitting to experimental results.
14. Computer-aided design/operation of the full-scale equipment and corresponding cost analysis.
15. Feasibility study by taking also into account the respective subsidies.
16. Scale up of column design to the next level.
17. Simulation of the production process under usual and expected extreme conditions.
18. Collection of the most likely to occur processing failures and consequent product defects.
19. Ranking of failures/defects in order of decreasing importance.
20. Fault Tree Synthesis (FTS) and selection of experts to assign significance indices or weights (in fuzzy version, to count for uncertainty) upon each cause-effect link/relation.
21. FTA and confirmation of ultimate causes found as most responsible for the top event.
22. Remedial proposals and testing of their effectiveness.
23. Development/operation/updating of an internal Knowledge Base (KB) and searching in external KBs for data mining by means of an Intelligent Agent, according to [4].

A. Are they adequate for modeling?
B. Is the goodness of fitting satisfactory at a pre-determined significance level?
C. Is the goodness of fitting satisfactory at the new significance level?
D. Is the goodness of fitting satisfactory at a pre-determined significance level?
E. Is the goodness of fitting satisfactory at the new significance level?
F. Are the results of the feasibility study in favor for the completion of the project?
G. Is there a next level in the scale up procedure?
H. Is there a next failure/defect ranked?

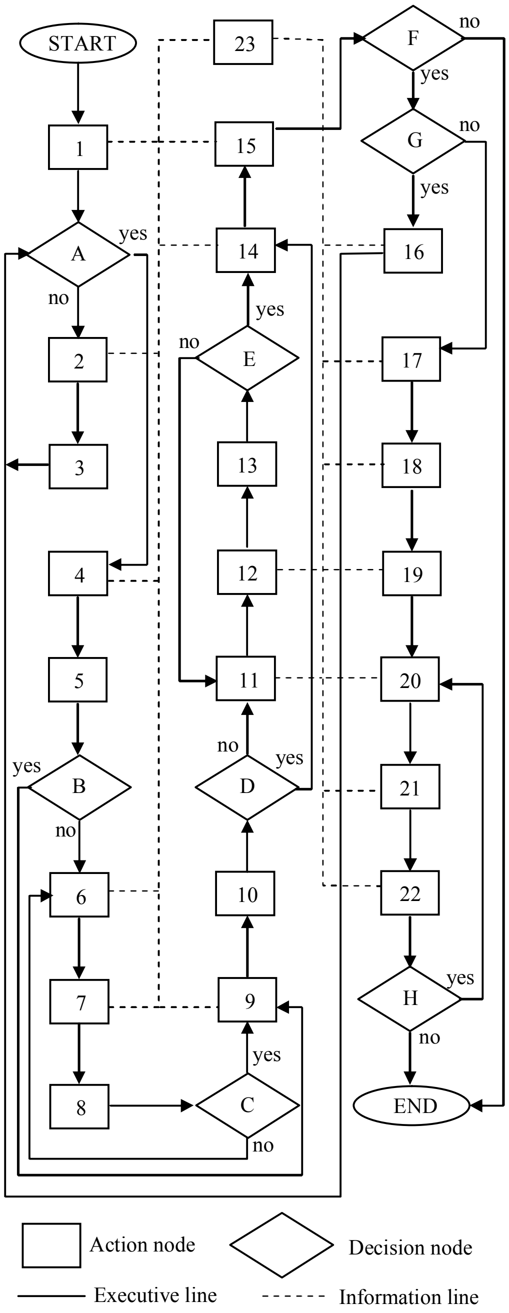

Fig. 2. The methodological framework, under the form of an algorithmic procedure, designed/ developed for determining enhanced quality of waste biomass modified to serve as a low cost substitute for activated carbon in packed bed adsorption columns.

3 Implementation

The fault tree synthesized for the implementation case example, i.e., "low rate of adsorption on pre-treated biomass", is presented in Fig. 3, whereas the description of the nodes is shown below. It is worthwhile noting that the higher-level causes for the top event (1.1 and 1.2) include both factual defects (i.e., defects that have been documented as stand-alone observations and/or through unfolded failure mechanisms) and misjudgment of features (i.e., overestimation of inherent potential), respectively, with a view to optimizing biomass quality via bridging the gap between theory-based-simulation and empirical-based modeling.

1.1 Real failure/defect, mainly at deep knowledge level.

1.2 Estimated reduction of adsorptiveness, mainly at surface knowledge level.

1.1.1 Devaluation before processing.

1.1.2 Devaluation during processing.

1.1.3 Devaluation after processing.

1.2.1 Imprecise measurement.

1.2.2 Unsuccessful determination/identification of variables/parameters influencing adsorptiveness.

1.2.3 Wrong/inadequate sampling and statistical analysis.

1.1.1.1 Deterioration before collection.

1.1.1.2 Deterioration during collection.

1.1.1.3 Deterioration after collection.

1.1.2.1 Improper conditions (e.g., temperature, pressure, composition of raw materials) in processing.

1.1.2.2 Low efficiency of additives.

1.1.3.1 Natural ageing due to endogenous reasons, according to the 2nd Law of Thermodynamics, especially in surface regions with high free energy resulted by very successful processing.

1.1.3.2 Accelerated ageing due to exogenous reasons, especially under conditions (e.g., high temperature/sunlight, humidity, microbial contamination) favoring enzymatic hydrolysis.

1.2.1.1 Low precision of the measuring instrument.

1.2.1.2 Invalid calibration.

1.2.3.1 Total underestimation because of low representativeness of the sample.

1.2.3.2 Local underestimation because of taking into account a great number of measurements (for sake of completeness) in the region of relatively low concentration of the adsorbate in solution (i.e., high concentration on the adsorbent surface) causing low fitting of the kinetic function to data in the region of high concentration of adsorbate (leverage effect).

1.1.1.1.1 Limited availability of collection machinery.

1.1.1.1.2 Limited availability of human resources.

1.1.1.2.1 Lack of proper machinery.

1.1.1.2.2 Lack of skilled personnel.

1.1.1.3.1 Shortage of space in warehouse.

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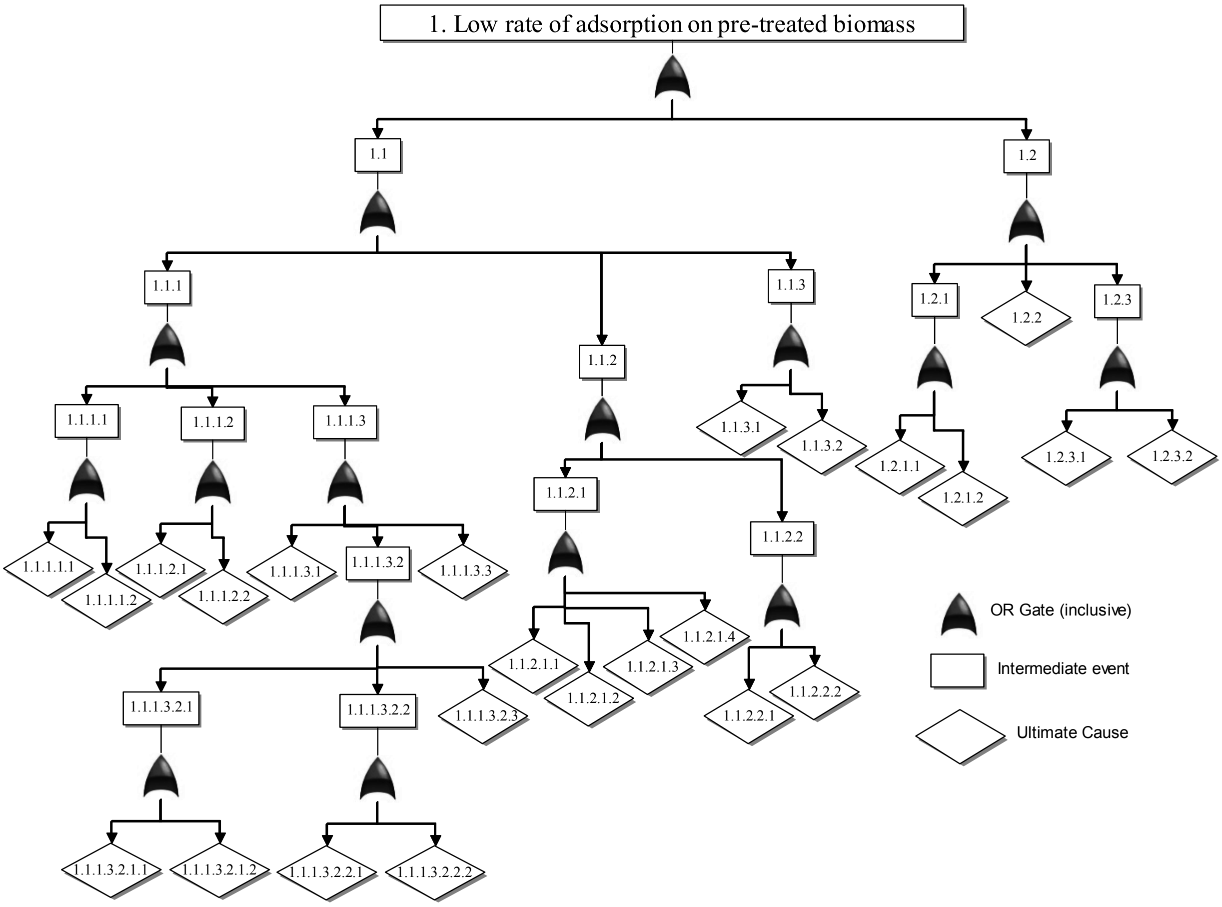

Fig. 3. The fault tree presented in the Section of Implementation without technical/quantitative details.

1.1.1.3.2 High detention time in warehouse due to increase of the [supply-demand] difference.
1.1.1.3.3 Improper micro-climatic conditions either at warehouse storage or at open air storage.
1.1.2.2.1 Improper kind or quality.
1.1.2.2.2 Uneven dispersion in the bulk of lignocellulosics under processing.
1.1.1.3.2.1 Incomplete information transfer to users.
1.1.1.3.2.2 Unsatisfactory market price of the downstream product.
1.1.1.3.2.3 Surplus supply of lignocellulosic waste.
1.1.1.3.2.1.1 Lack of proper communication with the users.
1.1.1.3.2.1.2 Lack of information at the required granularity level.
1.1.1.3.2.2.1 Low quality in comparison with competitive materials that may serve as substitutes.
1.1.1.3.2.2.2 Low market price of alternative raw materials available in the vicinity during the same season

The only logical gate used is the inclusive OR, since all the variables/nodes/events combine in the IF-part of each fuzzy rule by means of this gate that includes *a priori* the conjunctive AND-gate; on the other hand, the logical gate NOT is not used since it may introduce non-coherency into the FTA system according to [5].

A sample of fuzzy inference in the case under consideration is shown in Fig. 4, where the values of input-output variables are represented by triangular fuzzy numbers, i.e., the most likely to occur value corresponds to a point rather than to a region (in which case the fuzzy number is represented by a trapezoid). The input values (rounded to the nearest integer) are (68, 77, 81) for 1.1.3.1, (51, 60, 63) for 1.1.3.2, (53, 61, 67) for 1.1.1, (62, 66, 71) for 1.1.2, and (55, 64, 69) for 1.2. The estimated crisp values (after defuzzification, according to the centroid method) are 63.1667 for 1.1.3, 52.5556 for 1.1, and 86.4444 for the top event. All values are percentages of the corresponding indices.

4 Discussion and Conclusion

The final events, represented in Fig. 4 as rhombi, may not actually be ultimate causes, since they can

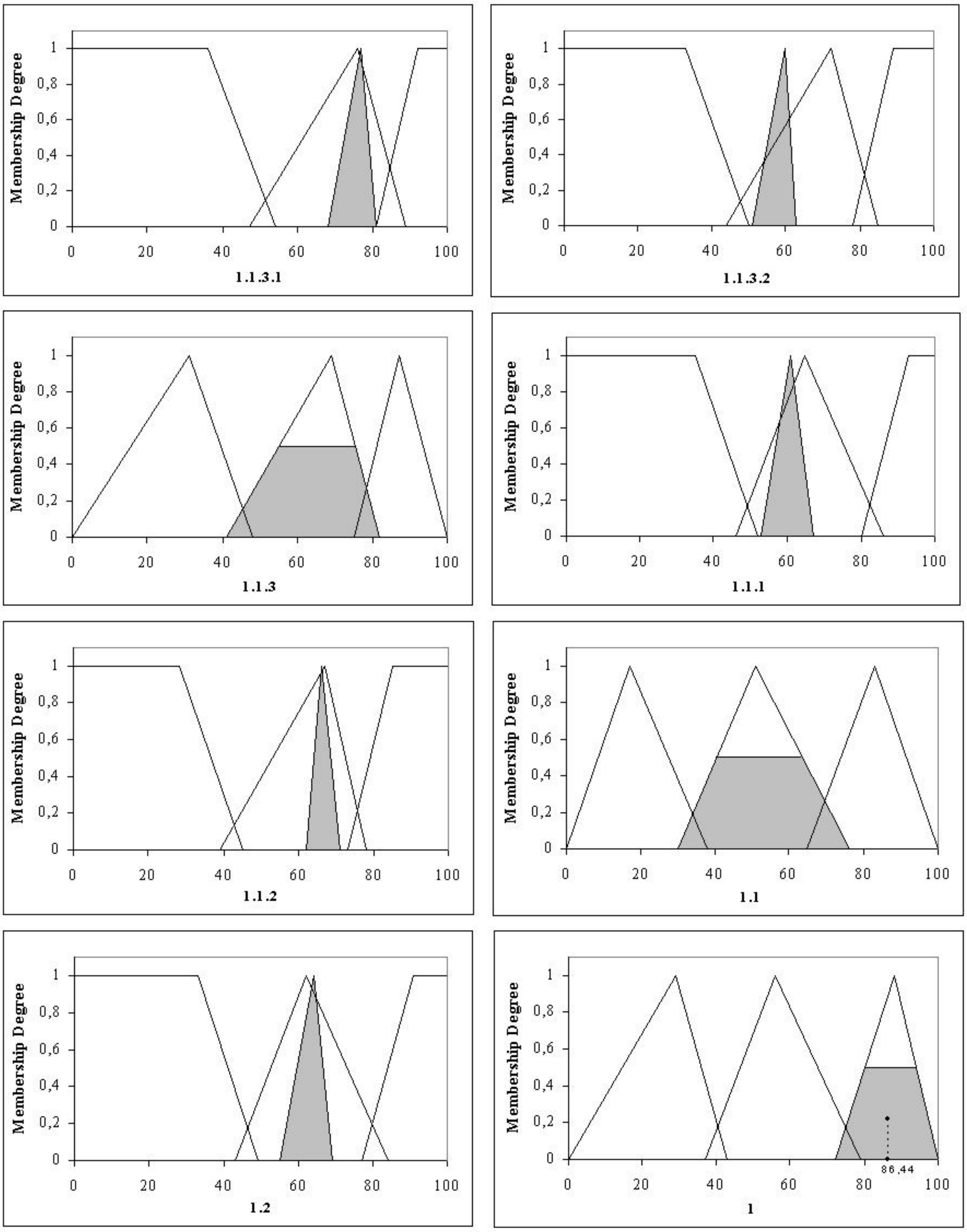

Fig. 4. Membership function of some of the variables/nodes (defined in the normalized 0-100 domain, after partitioning with the *Low*, *Medium*, *High* linguistic terms [6]) that participate within the fuzzy chain leading from the final events 1.1.3.1 (natural ageing due to endogenous reasons) and 1.1.3.2 (accelerated ageing due to exogenous reasons) to the top event 1 (low rate of adsorption on pre-treated biomass); the completely shadowed triangles are input fuzzy numbers while the shadowed trapezoids are estimated fuzzy numbers, giving the corresponding crisp numbers after defuzzification.

be further analyzed. For example, the node 1.1.3.2, taken as input variable in the inference example used for the implementation described above, may be further analyzed to 1.1.3.2.1: high temperature; 1.1.3.2.2: high solar radiation shifting to the ultraviolet (UV) part of the spectrum; 1.1.3.2.3: high

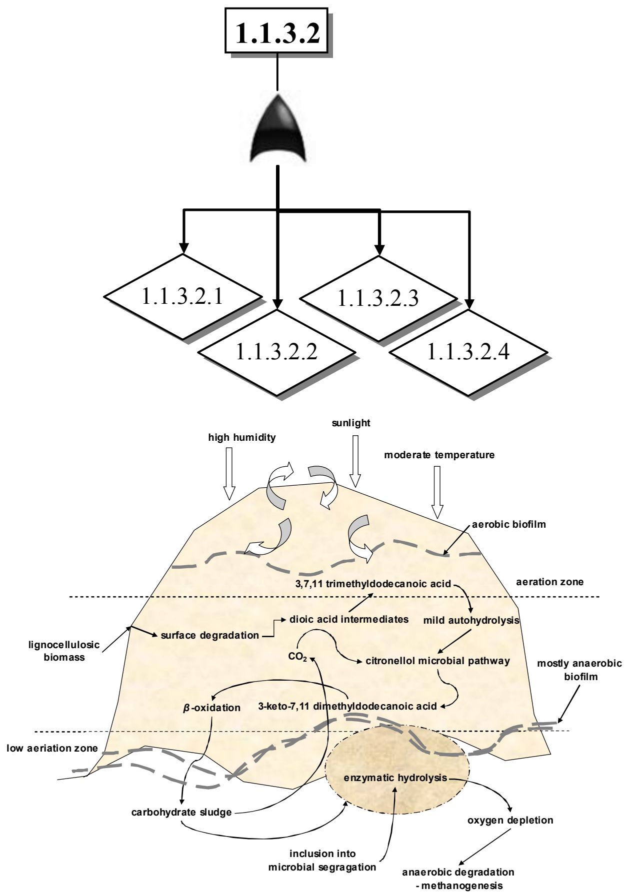

Fig. 5. Extending the node 1.1.3.2 (top diagram), referring to biomass ageing due to exogenous (environmental factors) to its ultimate causes that include the effects of temperature (1.1.3.2.1), sunlight (1.1.3.2.2), humidity (1.1.3.2.3) and microbial degradation (1.1.3.2.4). For example, the lignocellulosic residues pilling up at the edges of the fields are especially susceptible to decay (bottom diagram), occurring through a variety of complex and looped pathways that include mechanical, chemical and biochemical synergies, prohibited any further utilization of the biomass.

humidity; 1.1.3.2.4: high concentration of certain microbial species. Assignment of significant indices or weights on the causal relations between successive nodes of the chain leading to the top event presupposes deep knowledge of the interaction between these variables, which is rather complicate, as shown in Fig. 5. For engineering purposes, it is recommended to avoid such detailed analysis. Thus, the experts are asked to use their tacit/implicit knowledge in order to terminate searching in depth when marginal cost due to additional resources are higher than the expected marginal benefit from acquiring information at higher granularity level or corresponding knowledge at deeper phenomenological levels.

In conclusion, we have proved the functionality/ operability of the methodology we have designed/ developed, under the form of an algorithmic procedure, for determining enhanced quality of waste biomass modified to serve as a low cost substitute for activated carbon in packed bed adsorption columns. Moreover, the fuzzy FTA we have used for analyzing an implementation example showed the capability of the method to improve the efficiency of the process under consideration by synthesizing a fault tree as a direct problem presentation (top-down) and solving it as the inverse (bottom-up) problem.

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