THE 26TH EUROPEAN MODELING & SIMULATION SYMPOSIUM

SEPTEMBER 10-12 2014

BORDEAUX, FRANCE

EDITED BY

MICHAEL AFFENZELLER
AGOSTINO G. BRUZZONE
EMILIO JIMÉNEZ
FRANCESCO LONGO
YURI MERKURYEV
LIN ZHANG

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UPPER AUSTRIAN UNIVERSITY OF APPLIED SCIENCES, AUSTRIA
Michael.Affenzeller@fh-hagenberg.at

AGOSTINO BRUZZONE
MITIM-DIME, UNIVERSITY OF GENOA, ITALY
agostino@itim.unige.it

EMILIO JIMÉNEZ
UNIVERSITY OF LA RIOJA, SPAIN
emilio.jimenez@unirioja.es

FRANCESCO LONGO
DIMEG, UNIVERSITY OF CALABRIA, ITALY
f.longo@unical.it

YURI MERKURYEV
RIGA TECHNICAL UNIVERSITY, LATVIA
merkur@itl.rtu.lv

LIN ZHANG
BEIHANG UNIVERSITY, CHINA
zhanglin@buaa.edu.cn

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WELCOME TO EMSS 2014!

The European Modeling & Simulation Symposium (EMSS) is the traditional simulation appointment in Europe; indeed EMSS is also known as the *Simulation in Industry* Symposium due to the large participation of researchers as well as practitioners working in the area of Modeling & Simulation (M&S) applied to Industry and Industrial Engineering. To this end, EMSS 2014 has strongly confirmed its own nature; tracks such as Industrial Engineering and Industrial Processes Modeling & Simulation have collected very high quality scientific papers proposing advanced simulation applications and methodology approaches in multiple domains. However EMSS 2014 has also confirmed its capability to be a point of attraction for researchers working in other areas. Indeed, this edition of EMSS includes papers in the area of Discrete, Combined, Distributed and Parallel Simulation, Simulation and Artificial Intelligence, Modeling & Simulation in Physiology and Medicine (joint track with the International Workshop on Innovative Simulation for Health Care, IWISH 2014), Modeling & Simulation Approaches In and For Education as well as Modeling & Simulation Methodologies, Techniques and Applications. As chair of EMSS 2014 we would like to take this opportunity to thank all the authors and the reviewers of EMSS; their invaluable work is the key of the symposium success. We would like also to inform authors that, as every year, the EMSS 2014 proceedings will be indexed by SCOPUS.

As every year, EMSS is co-located with the International Multidisciplinary Modeling & Simulation Multiconference (I3M 2014) that this year includes six International Conferences (EMSS, HMS, MAS, DHSS, IWISH, SESDE) therefore providing EMSS attendees with the possibility to spend the three conference days in an extended simulation framework where people working in different areas, such as Logistics and Supply Chain, Defense and Homeland Security, Healthcare, Energy, Sustainable Development and Environment, share their simulation experiences. Finally, this year EMSS is held in the wonderful framework of Bordeaux, France; nothing is better than working and meeting old and new friends while drinking red Bordeaux!

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The EMSS 2014 International Program Committee (IPC) has selected the papers for the Conference among many submissions; therefore, based on this effort, a very successful event is expected. The EMSS 2014 IPC would like to thank all the authors as well as the reviewers for their invaluable work.
A special thank goes to all the organizations, institutions and societies that have supported and technically sponsored the event.

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APPLYING AN ADAPTIVE PETRI NET TO CALCULATE THE MAKESPAN IN THE JOB SHOP SCHEDULING PROBLEM

Joselito Medina-Marin[(a)], Juan Carlos Seck-Tuoh-Mora[(b)], Norberto Hernandez-Romero[(c)], Nayeli Jazmin Escamilla-Serna [(d)]

[(a,b,c,d)]Autonomous University of Hidalgo State, Advanced Research Centre in Industrial Engineering, Pachuca de Soto, Hidalgo, México

[(a)]jmedina@uaeh.edu.mx, [(b)]jseck@uaeh.edu.mx, [(c)]nhromero@uaeh.edu.mx, [(d)]nj_esser@hotmail.com

ABSTRACT

The Job Shop Scheduling Problem (JSSP) is one of the typical problems that engineers face on designing Flexible Manufacturing Systems (FMS). In this problem, it is important to find the optimal scheduling to perform a set of tasks in the minimum time. Moreover, the JSSP has some restrictions, such as the tasks order and the number of shared resources where the tasks are carried out. To find the optimal tasks sequence it is necessary to obtain the makespan for each sequence. On this way, FMS can be modeled with Petri nets (PNs), which are a powerful tool that have been used to model and analyze discrete event systems. So, the JSSP can be analyzed in a PN representation of the FMS, and the makespan can be calculated by using the PN model. In this work we propose an adaptive PN to obtain the makespan by applying PN analytical tools.

Keywords: job-shop scheduling problem, makespan, Petri nets, state equation.

1. INTRODUCTION

A Flexible Manufacturing System (FMS) is a discrete event dynamic system that is composed by jobs and shared resources (Zhou and Venkatesh 1999). The typical problem that engineers faced when they are either designing a Flexible Manufacturing System or planning the master production plan for the FMS, is how they should make the best sequence of jobs in the FMS in order to carry all operations out in the minimum time (Pinedo 2012; Lenstra 1977).

This problem is called the Job Shop Scheduling Problem (JSSP), which is a combinatorial problem classified as NP-Complete (Lenstra et al., 1977). There have been published several research papers about finding the minimum value of makespan in the JSSP (Shuai, and Zhi-Hua 2014; Qing-dao-er-ji, and Wang 2012; Zhao, Zhang, and Bing 2011; Ardakan, Hakimian, and Rezvan 2014). The makespan is the time that all the jobs are processed in the FMS, and it depends on the order that all the tasks are performed.

Several exact methods have been analyzed to find the minimum value for the makespan (Dey, Sarkar and Basu 2010; Wang, Cai, and Feng 2010; Wang and Zou 2003). These methods such as branch and bound, linear programming and Langrangian relaxation can find the global minimum value, however for problems with a bigger number of resources and jobs they need a huge amount of computational time to have the final result.

On the other hand, there are also research papers that apply meta-heuristics and/or evolutionary computing to find the minimum makespan time (Qing-dao-er-ji, and Wang 2012; Zhao, Zhang, and Bing 2011). In this case, these proposals can find reasonable results in less time than exact methods. The main drawback of these methods is that the global minimum could not be found, but good approximations are obtained in a short time.

FMSs have been modeled via Petri Nets (PNs) in order to simulate and analyze them. PN theory is adequate to represent in a graphical and mathematical way Discrete Event Systems (DES) such as FMSs, because their dynamic behavior based on event occurrence can be modeled by PN elements (places and transitions) (Murata 1989; Zhou and Venkatesh 1999). Moreover, PN theory offers analytical tools to study the modelled systems, based on the relationship among the FMS resources denoted as PN elements.

One important point in search methods is the calculus of the makespan, taking into account a certain processing order of the tasks. In this paper, we propose the use of an adaptive PN to calculate the makespan by means of the PN state equation.

2. JOB SHOP SCHEDULLING PROBLEM

Scheduling tasks in a FMS is a typical combinatorial problem where it is needed to organize the processing of a set of jobs divided in operations, and each operation is carried out in a shared resource (Gonzalez-Hernandez 2011; Quen-dao-er-ji and Wang 2012).

In the JSSP there are n jobs, and each job consists of m operations, and each operation is processed in a shared resource or machine during a fixed time. Some restrictions should be considered: operations of the same job have a sequence established previously, a job can visit each machine only once, each machine can

process only one job at any time, and there are not restrictions about the precedence among operations of different jobs.

The aim of JSSP is to find a sequence order for operation processing with the minimum value for the makespan.

For instance, Table 1 shows a FMS taken from (Zhang 2010) with some modifications to respect the JSSP restrictions. This example has three machines, four jobs, and each job has three serial operations.

Table 1: FMS configuration with operation times.

Items	Jobs	Operation Serial Number		
		1	2	3
Machine utilization	J_1	M_3	M_1	M_2
	J_2	M_2	M_3	M_1
	J_3	M_3	M_1	M_2
	J_4	M_2	M_1	M_3
Operation time	J_1	$O_{1,1,3}$ *96*	$O_{1,2,1}$ *90*	$O_{1,3,2}$ *35*
	J_2	$O_{2,1,2}$ *74*	$O_{2,2,3}$ *57*	$O_{2,3,1}$ *91*
	J_3	$O_{3,1,3}$ *13*	$O_{3,2,1}$ *5*	$O_{3,3,2}$ *7*
	J_4	$O_{4,1,2}$ *71*	$O_{4,2,1}$ *23*	$O_{4,3,3}$ *38*

Where $O_{i,j,k}$ denotes the *j*-th operation of the *i*-th job to be carried out by the *k*-th machine.

3. PETRI NETS CONCEPTS

A PN is a graphical and mathematical tool that has been used to model concurrent, asynchronous, distributed, parallel, non-deterministic, and/or stochastic systems.

The graph of a PN is directed, with weights in their arcs, and bipartite, whose nodes are of two types: *places* and *transitions*. Graphically, places are depicted as circles and transition as boxes or bars. PN arcs connect places to transitions or transition to places; it is not permissible to connect nodes of the same type. The state of the system is denoted in PN by the use of *tokens*, which are assigned to place nodes.

A formal definition of a PN is presented in table 2 (Murata 1989).

Table 2: Formal definition of a PN

A Petri net is a 5-tuple, $PN = (P, T, F, W, M_0)$ where:
$P = \{p_1, p_2, \ldots, p_m\}$ is a finite set of places,
$T = \{t_1, t_2, \ldots, t_n\}$ is a finite set of transitions,
$F \subseteq \{P \times T\} \cup \{T \times P\}$ is a set of arcs,
$W = F \rightarrow \{1, 2, 3, \ldots\}$ is a weight function,
$M_0 = P \rightarrow \{0, 1, 2, 3, \ldots\}$ is the initial marking,
$P \cap T = \varnothing$ and $P \cup T \neq \varnothing$.

The token movement through the PN represents the dynamical behaviour of the system. In order to change the token position, the following transition firing rule is used (Murata 1989):

1. A transition $t \in T$ is enabled if every input place $p \in P$ of t has $w(p,t)$ tokens or more. $w(p,t)$ is the weight of the arc from p to t.
2. An enabled transition t will fire if the event represented by t takes place.
3. When an enabled transition t fires, $w(p,t)$ tokens are removed from every input place p of t and $w(t,p)$ tokens are added to every output place p of t. $w(t,p)$ is the weight of the arc from t to p.

A Timed Place Petri Nets (TPPN) is an extended PN, where a new element is added. It is a six-tuple $TPPN = \{P, T, F, W, M_0, D\}$, where the first fifth elements are similar to PN definition presented above, and $D = \{d_1, d_2, \ldots, d_m\}$ denotes the time-delay for each place $p_j \in P$ (Zhao, Zhang, and Bing 2011). Output transitions t_i for each p_j will be enabled once the time indicated in p_j is reached.

3.1. Analysis methods

In this paper, we are applying the matrix equation approach as the analytical method of PN theory in order to calculate de makespan of the FMS modelled.

3.1.1. Incidence matrix and state equation

A *PN* with n transitions and m places can be expressed mathematically as an $n \times m$ matrix of integers $A = [a_{ij}]$. The values for each element of the matrix are given by: $a_{ij} = a_{ij}^{+} - a_{ij}^{-}$, where a_{ij}^{+} is the weight of the arc from t_i to p_j, and a_{ij}^{-} is the weight of the arc from p_j to t_i.

The state equation is used to determine the marking of a *PN* after a transition firing, and it can be written as follows:

$$M_k = M_{k-1} \times A^T U_k, \text{ k=1,2,…} \quad (1)$$

where u_k is a $n \times 1$ column vector of n - 1 zeros and one nonzero entries, which represents the transition t_j that will fire. The nonzero entry is located in the position j of u_k. A^T is the transpose of incidence matrix. M_{k-1} is the marking before the firing of t_j. And Mk is the reached marking after the firing of t_j denoted in u_k.

4. ADAPTIVE TIMED PLACE PETRI NET

In this paper we propose an adaptive TPPN (ATPPN), which adds some arcs according to tasks sequence of the FMS.

The formal definition of an ATPNN is as follows: An ATPNN is a seven-tuple $(P, T, F, W, M_0, D, F_d)$, where the first six elements are similar to TPNN elements, and the last one, F_d, is the set of dynamic arcs that change depending on the job operations order. $F_d \subseteq \{P \times T\} \cup \{T \times P\}$. $F \cap F_d = \varnothing$.

4.1. One operation modelling

The ATPNN to model one operation O_{ijk} of a job J_i processed by machine M_k is depicted in figure 1.

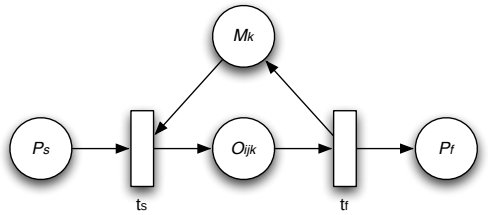

Figure 1: Operation O_{ijk} processed by machine M_k denoted as a PN model.

4.2. One job modelling

As we mentioned above, one job J_i is composed of operations O_{ijk}, so the PN model for each J_i is a concatenation of its operations O_{ijk} (Figure 2).

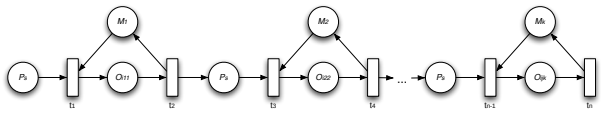
Figure 2: Operations O_{ijk} of job J_i processed by machines M_k denoted as a PN model.

4.3. FMS modelling

In order to model the whole FMS, we add the PN structure for each job J_i and connect every M_k place with its corresponding input (output) transition from (to) operation O_{ijk}. Figure 3 shows the PN model for the FMS described in Table 1.

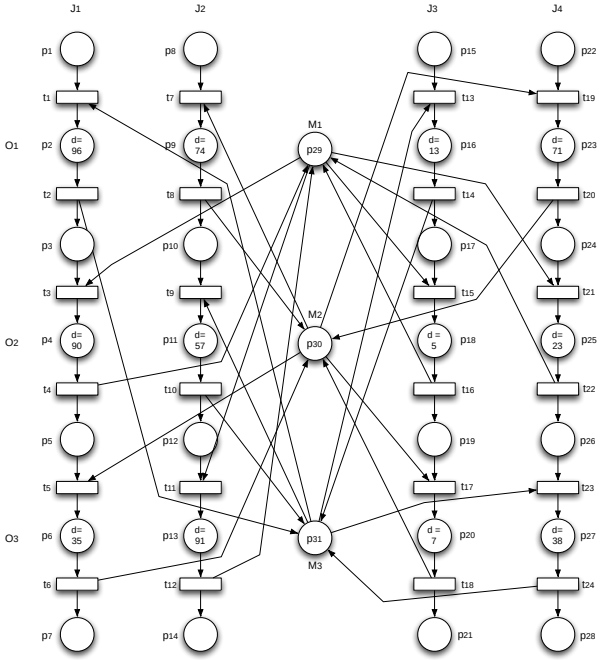

Figure 3: PN model for the FMS described in Table 1.

In Figure 3, each column corresponds to each job J_i, and some places have a label *d*, which denotes the time delay for processing an operation O_{ijk} in the connected machine M_k.

4.3.1. Algorithm to convert a TPPN into an ATPPN

At this time, PN model of figure 3 only represents the FMS, but it is also necessary to set the priority in the operations processing by means of arcs connection in the PN model. So, we need to define the elements of F_d to denote this priority.

First of all, the operations sequence is defined in a row vector $OS = [os_1\ os_2\ \dots\ os_{i\times j}]$, where each *OS* value corresponds to one operation O_{ijk}. The following algorithm receives as inputs the row vector OS and the TPPN model, as output of the algorithm we obtain the ATPPN.

Algorithm `TTPN_into_ATPPN`
Input: `TPPN, OS`
Output: `ATPPN`

```
1. For q=1 to i×j
    k = machineOf(OS(q))
    add(MO(k),OS(q))
End For
2. For k = 1 to NumberOfMachines
    For i = 1 to NumberOfJobs - 1
        p1 = placeOf(MO(k,i))
        p2 = placeOf(MO(k,i+1))
        t1 = p1•
        t2 = •p2
        p3 = •t2
        W(t1, p3) = 1
        W(p3, t2) = 2
    End For
End For
```

In Step 1, a $k\times i$ matrix called M_O is created. Operations $os \in OS$ (O_{ijk}) carried out by the same machine M_k are added in the row k of M_O. The sequence order for the same machine is taking into account.

In Step 2, new arcs $(t,p) \in F_d$ are created, which connect output transitions of places representing operations O_{ijk} with the input place of next operation O_{ijk} in the sequence order defined in M_O. Moreover, a value 2 is assigned to weight $W(p_3,t_2)$, to assure the order in the operations processing.

To illustrate the algorithm result, figure 4 shows the ATPPN obtained, based on the operations denoted in figure 3 and following the order: $OS = [O_1J_2,\ O_1J_4,\ O_2J_2,\ O_1J_3,\ O_2J_4,\ O_1J_1,\ O_3J_2,\ O_3J_3,\ O_2J_1,\ O_3J_1,\ O_2J_3,\ O_3J_3]$.

The ATPPN model presented in figure 4 is used to calculate the makespan for the sequence defined in vector *OS*.

5. ALGORITHM TO OBTAIN THE MAKESPAN

The proposed algorithm takes into account the mathematical representation of the ATPPN. In particular, the incidence matrix and the state equation are utilised to obtain the time delay for each O_{ijk}.

As input data the algorithm needs the ATPPN which includes its input arcs matrix (a_{ij}^-), the output arcs matrix (a_{ij}^+), the time delays column vector *D*, and the initial marking M_0, the total number of jobs (*nj*), the total number of operations per job (*no*), and the total number of shared machines (*nm*).

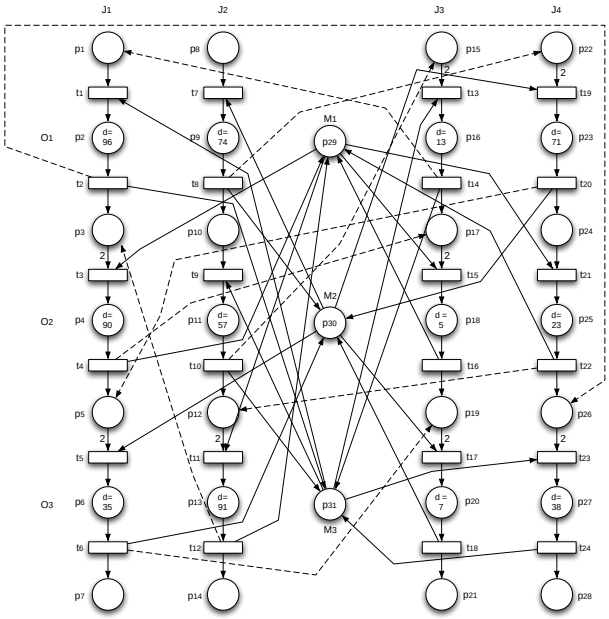

Figure 4: ATPPN model obtained applying the algorithm TTPN_into_ATPPN.

Algorithm Calculate_Makespan

Input: ATPPN, a_{ij}^-, a_{ij}^+, D, M_0, nj, no, nm

Output: *makespan*

1. Initialise variables:
   - txj = |T| / nj
   - pxj = (|P| - nm) / nj
   - AT = [0 0 … 0]' $_{|P| \times 1}$
   - TV = [0 0 … 0] $_{1 \times (nj)}$
2. ET = enabledTransitions(M_0, a_{ij}^-)
3. ∀et ∈ ET, U_k (et) = 1
4. While |ET| > 0
   - For each t ∈ ET
     - indexT = ceil(t/txj)
     - Uk_{tmp}^T = [0 0 … 0]' $_{|T| \times 1}$
     - Uk_{tmp}(t) = 1
     - τ = D' × (a_{ij}^-)' × Uk_{tmp}
     - τ_{accum} = AT' × (a_{ij}^-)' × Uk_{tmp}
     - max_τ_{accum} = max(TV(indexT), τ_{accum}/2) + τ
     - For each p ∈ $t^\bullet$
       - indexP = ceil(p/pxj)
       - If indexT == indexP
         - TV(indexP) = max_τ_{accum}
       - Else
         - AT(p) = max_τ_{accum}
       - End if
     - End For
   - End For
   - M_i = M_{i_1} + (a_{ij})' * Uk
   - ET = enabledTransitions(M_i, a_{ij}^-)
   - Uk^T = [0 0 … 0]' $_{|T| \times 1}$
   - ∀et ∈ ET, Uk(et) = 1
5. End While
6. makespan = max(TV)

In step 1, four variables are initialised: the number of transitions per job (*txj*), the number of places per job (*pxj*), a column vector AT to assign the accumulative time for each place, and a row vector TV utilised to save the time used for each job.

Step 2 obtains the enabled transitions (ET) for an initial marking M_0. Step 3 creates the *Uk* vector from ET transitions.

Step 4 makes an iterative process while the ATTPN is alive, i.e., while there exists at least one enabled transition in the current marking. So, for every enabled transition *t*, we identify the job J_i where the transition belongs (indexT), initialise a temporal *Uk* (Uk_{tmp}) to fire transition t. The time delay τ corresponding to current operation O_{ijk} is calculated multiplying the transpose of the time delay vector D' by the transpose of the input arcs matrix (a_{ij}^-), and the result is multiplied by the firing vector Uk_{tmp} taking into account only transition t.

The accumulated time, denoted as τ_{accum}, represents the time that the needed machine M_k has been busy previous to the current operation O_{ijk}. And it is calculated in a similar way that τ, but in this case we use an auxiliary vector *AT* where the accumulative time for each place is stored, instead of the time delay vector *D*.

Then, we compare both times, the time when the machine *Mk* is ready and the time when the operation O_{ijk} is also ready to be processed. The maximum time plus the time delay for operation O_{ijk} is assigned to max_τ_{accum}. For every $p \in t^\bullet$, if *p* and *t* are in the same job line then max_τ_{accum} is assigned to the time vector variable *TV*. On the other hand, if *p* and *t* belong to different job lines, max_τ_{accum} is assigned to the vector *AT*.

Finally, the ATPPN marking M_i changes according to the result of the equation state. From this new marking M_i, the new enabled transitions are assigned to vector ET and vector *Uk* is generated from them.

6. APPLICATION EXAMPLE

In order to show the applicability of this approach, the FMS configuration showed in Table 1 is taken. This FMS has four jobs, and each job is divided in three operations performed in three different machines.

Operation times showed in Table 3 come from the transposed matrix corresponding to operation times from Table 1.

Table 3: Processing time for each operation per job.

Operation serial number	J_1	J_2	J_3	J_4
1	96	74	13	71
2	90	57	5	23
3	35	91	7	38

Furthermore, to identify every operation in the whole FMS, an operation number was assigned to each one. (Table 4).

Table 3: Number assigned to each operation.

Operation serial number	J_1	J_2	J_3	J_4
1	1	4	7	10
2	2	5	8	11
3	3	6	9	12

Finally, the machine utilization in the FMS is showed in Table 5.

Table 5: Machine utilization.

Operation serial number	J_1	J_2	J_3	J_4
1	3	2	3	2
2	1	3	1	1
3	2	1	2	3

Based on the operation numbers from Table 4, we take the following operation sequence: *OS* = (4 10 5 7 11 1 6 12 2 3 8 9), which is a valid sequence.

From this sequence, the algorithm TPPN_into_ATPPN is executed which has as input data the operation sequence *OS* and the TPPN of figure 3, obtaining as output the ATPPN showed in figure 4. The dashed arcs represent the sequence of the machine operation on the PN model.

Next, the algorithm Calculate_Makespan needs the following data:

1. ATPPN (figure 4)
2. a_{ij}^{+} (figure 4)
3. a_{ij}^{-} (figure 4)
4. $D_{31\times1}$, is a column vector with 31 elements, denoting the processing time in the corresponding place (figure 4). For instance, place p_2 is holding a processing time of 96 time units, so D(2) = 96, which represents the operation time of machine 3 for the operation number 1 (Table 4), and so on.
5. M_0 is the initial marking, where $M_0(i) = 1$, for $i = 1,8,15,22,29,30,31$. And $M_0(j) = 0$ for $j \neq i, 1 \leq j \leq 31$. This marking denotes the starting of FMS operations (p_1, p_4, p_{15}, p_{22}) and the availability of the machines M_1, M_2 and M_3 (p_{29}, p_{30}, p_{31}).
6. $nj = 4$ (number of jobs)
7. $no = 3$ (number of operations per job)
8. $nm = 3$ (number of machines)

Under these conditions, the algorithm Calculate_Makespan starts the transition firing and the token game animation. In order to obtain the processing time for each transition that is fired, the Eq. (2) is computed.

$$\tau = D' \times a_{ij}^{-'} \times u_k \qquad (2)$$

The accumulated time for each job line is saved in vector $TV_{1\times4}$. Table 6 shows the TV values for each transition firing. There are some cases where two transitions were fired simultaneously.

Table 6: Time vector state after transition firings.

Transitions fired	*Time Vector (TV)*			
	J_1	J_2	J_3	J_4
t_7	0	0	0	0
t_8	0	74	0	0
t_9 t_{19}	0	74	0	74
t_{10} t_{20}	0	131	0	145
t_{13} t_{21}	0	131	131	145
t_{14} t_{22}	0	131	144	168
t_1 t_{11}	144	168	144	168
t_2 t_{12}	240	259	144	168
t_3 t_{23}	259	259	144	240
t_4 t_{24}	349	259	144	278
t_5 t_{15}	349	259	349	278
t_6 t_{16}	384	259	354	278
t_{17}	384	259	384	278
t_{18}	384	259	**391**	278

At the end, the maximum value of *TV* (391 time units) represents the makespan for this operation sequence.

The Gantt chart obtained, is showed in figure 5, where the maximum time is 391 time units. The value *#n* over each bar denotes the operation number assigned in Table 4.

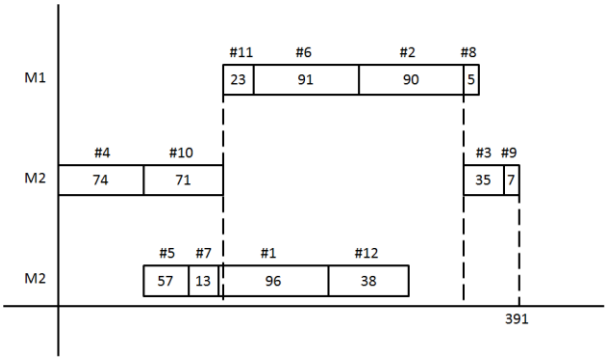

Figure 5: Scheduling chart Gantt for the operation sequence (4 10 5 7 11 1 6 12 2 3 8 9).

The makespan obtained from the scheduling Gantt chart is equal to the makespan obtained from the proposed approach.

7. CONCLUSIONS AND FUTURE WORK

JSSP is a NP-hard problem that has been analysed applying different kinds of techniques, such as exact models and heuristics strategies. One important calculus in the JSSP is the makespan value, which depends on the sequence of operations for each job and the order of machine utilisation.

In this paper, we propose a different way to calculate the makespan by means of mathematical tools

of Petri nets, such as the equation state and the incidence matrix. Firstly, we describe an algorithm to create an ATPPN from a FMS description. The ATPPN arcs indicate the order in which operations O_{ijk} must be done in each job. Moreover, arcs are connected adequately to set the operations order for each machine. And secondly, the marking evolution by using the state equation is taken into advantage to calculate the makespan. We added a time delay vector in order to consider the processing time for every operation involved in the FMS, and it is included in the matrix operations to be able to obtain the makespan for each job.

As future work, we are including these algorithms as part of a study based on evolutionary computing. Moreover, we are interested in analyse the feasibility of PN tools as part of an heuristic to obtain de minimum makespan in the JSSP.

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AUTHORS BIOGRAPHY

Joselito Medina-Marin. He received the M.S. and Ph.D. degrees in electrical engineering from the Research and Advanced Studies Centre of the National Polytechnic Institute at Mexico, in 2002 and 2005, respectively. Currently, he is a Professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State at Pachuca, Hidalgo, México. His current research interests include Petri net theory and its applications, active databases, simulation, and programming languages.

Juan Carlos Seck-Tuoh-Mora. He received the M.S. and Ph.D. degrees in electrical engineering (option: Computing) from the Research and Advanced Studies Centre of the National Polytechnic Institute at Mexico, in 1999 and 2002, respectively. Currently, he is a Professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State at Pachuca, Hidalgo, México. His current research interests include cellular automata theory and its applications, evolutionary computing and simulation.

Norberto Hernandez-Romero. He received the M.S. degree from Department of Electrical Engineering, Laguna Technological Institute at México, in 2001 and the Ph. D. from Autonomous University of Hidalgo State at México in 2009. Currently, he is a professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State at Pachuca, Hidalgo, México. His current research interests include system identification, feedback control design, genetic algorithms, fuzzy logic, neural network and its applications

Nayeli Jazmin Escamilla-Serna. She is a postgraduate student in Industrial Engineering in the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State at Pachuca, Hidalgo, México.

MODELING AND OPTIMIZATION OF THE EXTRACTION OF LIGNOSULFONATE FROM BARLEY STRAW BY USING ARTIFICIAL NEURAL NETWORKS

Maria Guadalupe Serna-Diaz[(a)], Joselito Medina-Marin[(b)], Ainhoa Arana-Cuena[(c)], Juan Carlos Seck-Tuoh-Mora [(d)], Alejandro Tellez-Jurado[(e)], Yuridia Mercado-Flores [(f)], Angelica Jimenez-Gonzalez[(g)], Norberto Hernández-Romero [(h)]

[(a)(c) (e) (f) (g)] Polytechnic University of Pachuca, Pachuca de Soto, Hidalgo, México
[(b) (d) (h)] Autonomous University of Hidalgo State, Advanced Research Centre in Industrial Engineering, Pachuca de Soto, Hidalgo, México

[(a)]sedg0210@yahoo.com.mx, [(b)]jmedina@uaeh.edu.mx, [(c)]ainhoa@upp.edu.mx, [(d)]jseck@uaeh.edu.mx, [(e)]alito@upp.edu.mx, [(f)]yuridiamercado@upp.edu.mx, [(g)]ajimenez@upp.edu.mx, [(e)]nhromero@uaeh.edu.mx

ABSTRACT
Artificial Neural Networks (ANNs) have been applied to model dynamic systems from a wide range of areas. In particular, we are interested in the application of ANN in fitting data sets to model the extraction process of lignosulfonates from barley straw. In order to know real data about the percentage of delignification taking into account three variables from the experimental process: cooking time of the barley straw, percentage of sulfite concentration applied to the barley straw, and barley size. With the data gathered from 75 experiments performed three times each one, we created an ANN optimal with a minimum mse, and we calculate an optimal value from this ANN model.

Keywords: Artificial neural network, Optimization, Lignosulfonate extraction, Data fitting.

1. INTRODUCTION

Lignocellulosic biomass is considered as a key element to avoid the fossil fuel dependence and encourage the use of raw material friendlier with the environment (Zhu, Sun, Su, Zhao, Ma, Zhu, Shi, and Gu, 2013).

The lignocellulosic biomass decomposition is based on three main compounds: cellulose, hemicellulose and lignin, which are joined in microfibrillar grouped in a chain of crystalline cellulose, covered with structures of hemicellulose and holocellulose protected by lignin (Abud, Costa, Wanderley, Souza, and Sant'Anna 2013). Nevertheless, these biopolymers are better utilized individually (Kahar, Taku, and Tanaka 2013).

Lignocellulosic material has a broad range of applications, but the use of each compound depends on the treatments utilized to extract them and how easy and cheap is the separation of the three compounds. These treatments can be physical (Subhedar and Gogate 2014; Iskalieva, Yimmou, Gogate, Horvath, Horvath, and Csoka 2012), chemical (Yang, Kuittinen, Zhang, Keinänen, and Pappinen, 2013; Duque, Manzanares, Ballesteros, Negro, Oliva, Saez, Ballesteros, 2013) or biological (El-Zawawy, Ibrahim, Abdel-Fattah, Solimanb, Mahmoud, 2011; Wang, Manley, and Feldmant, 2011).

Nowadays, the utilization of biomass extracted from agricultural residuals is often applied to obtain polymers. In the case of Barley (*Hordeum vulgare*), one kilogram of barley corresponds to 0.750 of straw (Carrera and Mateo 2005). For this reason, barley straw is a good option for extracting Lignocellulosic material (Singh, Shukla, Tiwari, and Srivastava, 2014). Moreover, lignin has many applications in industry, such as dispersant agent for mixture of cement and gypsum (Stráněl and Sebök, 1997), as emulsifier (Weis and Bird, 2001), in polymers production (Effendi, Gerhauser, and Bridgwater, 2008), and a new trend is the use of lignin in agricultural industry as soil conditioner (Deng et al., 2011) and vegetal growth promoter (Ertani et al., 2011).

The applications mentioned above utilize the lignin in the form of lignosulfonate (LS), which is the sulfonate lignin obtained from the separation with sulfite (Chakrabarty, Saha, and Ghoshal 2009). This process requires high temperature and pressure in order to depressurize the fibers of cellulosic material and reach its disaggregation. Furthermore, it is important to consider the size of the biomass (pieces of barley straw) and the concentration of the sulfite to find the maximum performance of delignification.

In this research work we took into account three independent variables: barley straw size, sulfite concentration, and cooking time. And as dependent variable we considered the performance percentage of delignification.

Experimental results were fitted through an Artificial Neural Network model in order to find an optimal combination of values that produce the maximum delignification performance.

2. MATERIALS AND METHODS

The lignocellulosic material of barley straw utilized in this work was taken from crops located in Zempoala, Hidalgo, Mexico. The separation was carried out in a semi-industrial autoclave AV-3580 Prendo®, which was modified to be able to reach 3 atm of pressure.

2.1. Variables

The variables for this experiment were: size of straw with a sieve number 8 (2.0 mm), 10 (1.68 mm) and 20 (0.84 mm); cooking time was 15, 30, 45, 60, and 90 minutes; finally, sodium sulfite concentrations with values of 1%, 3%, 5%, 10%, and 15%. The temperature was kept at 137 ºC, the pressure at 3 atm, and the relation between straw and sulfite was 1 part of straw for 25 of liquor. Then, a total of seventy five lab experiments were done ($3 \times 5 \times 5 = 75$). Table 1 shows the combination values for each experiment.

Table 1: Combination of values for each experiment

Experiment number	Sieve number	Cooking time	Sulfite concentra-tion
1	8	15	1
2	8	15	3
…	…	…	…
6	8	30	1
7	8	30	3
…	…	…	…
26	12	15	1
27	12	15	3
…	…	…	…
31	12	30	1
32	12	30	3
…	…	…	…
51	20	15	1
52	20	15	3
…	…	…	…
56	20	30	1
57	20	30	3
…	…	…	…
74	20	90	10
75	20	90	15

2.2. Lab experimental method

The straw was ground to separate the fibers. It was winnowed with chain mails of 8 (2.0 mm), 10 (1.68 mm) and 20 (0.84 mm). Then, 2g of straw for each size were mixed with 100 mL of sodium sulfite, in different concentrations (1%, 3%, 5%, 10%, and 15%). Every experiment was done in triplicate.

The digestive process was carried out in a closed system inside glass bottles and the cooking process was done in an autoclave with temperature of 137 ºC and pressure of 3 atm, during 15, 30, 45, 60, and 90 minutes. From this process, the cellulose pulp and the "liquor" were produced. Lignosulfonates contained in the liquor were separated by means of vacuum filtration, in filter paper with pore of 1.6 μm.

To quantify the solubilized material, the material retained by the filter paper was burned at 550 ºC during 6 hours. Then, the counting was done by weight difference, with a previous correction of the humidity and solubilized material in a sample without sulfite only with water (Northey, 1992; Ekeberg, Gretland, Gustafsson, Braten, and Fredheim, 2006).

The performance of delignification material is calculated with Equation 1.

$$PSM = \frac{DWs - (DWf - A - W)}{DWs} \cdot 100 \quad (1)$$

Where:
PSM: is the percentage of solubilized material.
DWs: is the initial dry weight.
DWf: is the final dry weight.
A: are the residual ashes.
W: is the sample without sulfite (only water).

2.3. Data fitting method

The data fitting was done through an Artificial Neural Networks (ANNs), which was trained, validated and tested with the 75 experimental results from the combination of 3 sizes of barley straw, 5 cooking times, and 5 sulfite concentrations.

2.3.1. Artificial Neural Network

An ANN is computational technique that performs a multifactorial analysis. It is inspired in biological neural networks, and is composed of nodes distributed in layers, and interconnected through lines with assigned weights.

Nodes represent artificial neurons, which are processing units performing a no-linear sum (Dayhoff, and Deleo, 2001). Connections weights are adjusted according to a training process of the ANN. An adequate training produces an ANN that helps in values forecasting, objects classification, function approximation, pattern recognition with multifactorial data, and modeling and optimization of data fit for different phenomena (Sinhaa, Chowdhurya, Sahaa, and Dab, 2013; Aghav, Kumar, and Mukherjee, 2011; Duque, Manzanares, Ballesteros, Negro, Oliva, Saez, and Ballesteros, 2013; Maache-Rezzoug, Pierre, Nouviaire, Maugard, and Rezzoug, 2011), among other applications.

In this work, we applied the Matlab® Neural Network Toolbox to perform the data fitting. The ANN model was obtained through an iterative process. In it we were changing the number of neurons, and the ANN model was trained ten times, saving the ANN with the less Mean Square Error (mse). The method used for

training was the Levenberg-Marquardt method, and the data division for training, validating, and testing was done randomly.

3. RESULTS

3.1. Lab experimental results

Results obtained from straw delignification with different values for sulfite concentration, cooking time, and size of barley straw are showed in figure 1.

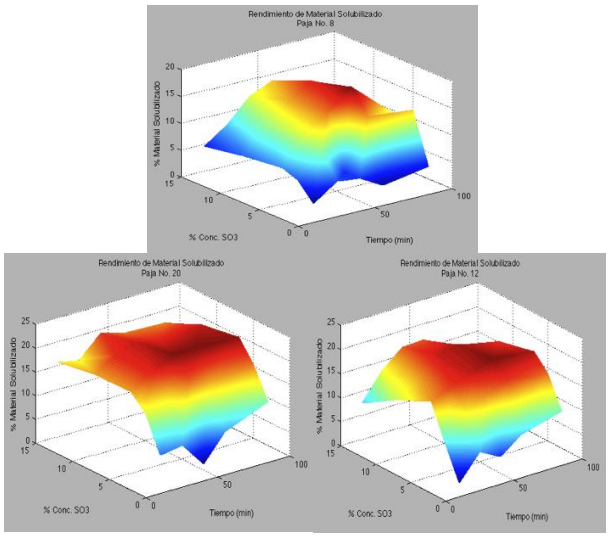

Figure 1: Percentage of solubilized material from straw barley of size 8(a), 12(b) and 20(c).

The lower percentages of delignification are represented by dark blue color and the higher percentages are represented by dark red color.

Figure 1 shows that the maximum value of percentage of delignification is located in the same value for cooking time (60 minutes) and sulfite concentration (5%) for each value of barley straw size. For the barley straw size 8, the maximum value is 18.7 ± 0.53, for size 12 the maximum value is 20.4 ± 0.47, and for size 20 the maximum value is 22.5 ± 1.3.

3.2. ANN model results

The data fitting was performed through an ANN model, which was created with the Neural Network Toolbox included in Matlab®.

Furthermore, a Matlab® script was implemented to find an ANN model with a minimum mse. This script creates ANN models starting from a model with 3 layers; the first one considers the three input variables (barley straw size, cooking time, and sulfite concentration); the second one is the hidden layer where the connections weights are set from the training process; and the last layer contains only one neuron with the value of the percentage of solubilized material.

70% of the experimental data (56 samples) were utilized in the training process, and they were chosen randomly. 15% of the data (11 samples) were utilized to validate the model, and the other 15% (11 samples) of data were utilized to test the ANN model.

The ANNs created in the scritp were trained with the Levenberg-Marquardt backpropagation algorithm, and we iterate from an ANN with 3 neurons until an ANN with 50 neurons. Each one was trained ten times in order to find a model with the minimum mse.

Taking into account this criterion, we found an ANN model with 20 neurons and the less mse of 1.2214 (Figure 2).

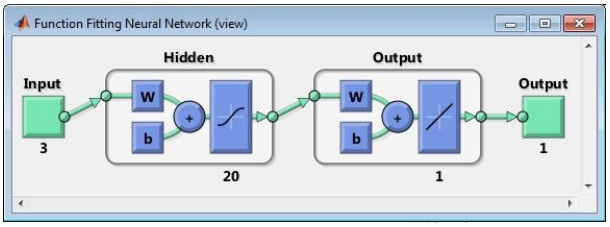

Figure 2: ANN model with minimum mse.

Figure 3 contains the graphic for lab experimental data and the data obtained from the ANN model. The seventy five values obtained from lab experiments are denoted as small red circles, and the dashed line denotes the data forecasted from the ANN model, for the same seventy five combinations. The axis of abscissas represents the experiment number, where each experiment was performed in a combination of values for sieve number, cooking time, and sulfite concentration. The axis of ordinates indicates the percentage of solubilized material obtained from each combination.

The model showed in figure 2 was utilized to estimate the parameters for the optimal value of percentage of delignification. The input value for barley straw size was iterated from 8 to 20, the input value for cooking time was iterated from 15 to 90 minutes, and the input value for sulfite concentration was iterated from 1 to 15. Each parameter was incremented in steps of one, and we obtained a total of 14 820 combinations in order to evaluate the ANN model for each one.

The highest value of solubilized material calculated with this ANN model was 24.6432%, with barley straw size of 16, a cooking time of 42 minutes, and a sulfite concentration of 15%.

Figure 4 shows the graphic generated with all the data forecasted with the ANN model. As in figure 3, the small red circles denotes the seventy five lab experimental data, and the green graphic denotes the 14 820 forecasted data from the ANN model. Similar to figure 3, the axis of abscissas represents the experiment number, and the axis of ordinates indicates the percentage of solubilized material.

The circle filled in red indicates the optimal value of solubilized material.

4. CONCLUSIONS

Lignocellulosic material has been applied in different areas, and it has been gotten from different sources. Currently, agricultural residuals are used to extract lignin with good results.

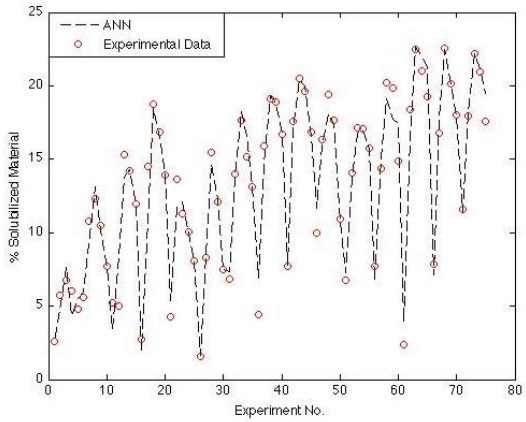

Figure 3: Comparative graphic between experimental data and data predicted with the ANN model.

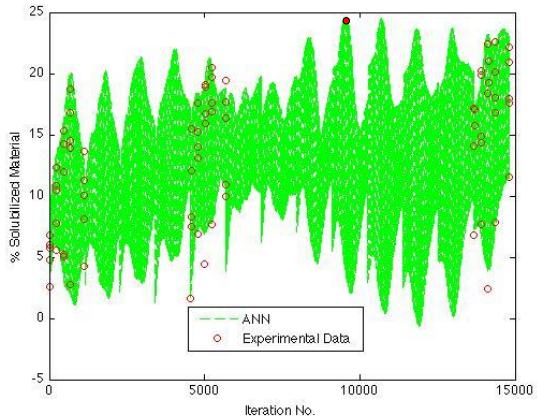

Figure 4: optimal value found in all the data forecasted with the ANN model.

In this work, we used barley straw to get lignin from biomass, and to analyze the effect of factors as barley straw size, cooking time, and sulfite concentration, a total of 75 experiments were carried out. The three barley straw sizes considered were 8, 12, and 20; the five cooking times utilized were 15, 30, 45, 60, and 90 minutes; and the five sulfite concentrations were 1%, 3%, 5%, 10%, and 15%.

Experimental data were used to create ANNs with different number of neurons and trained ten times. The ANN with the lower mse (1.2214) was taken to search the optimal value for percentage of delignification. The maximum value found for the solubilized material with the ANN model was 24.6432%, for a barley straw size of 16, cooking time required of 42 minutes, and sulfite concentration of 15%.

As future work, we are going to take into account some economic considerations, in order to estimate the cost for producing lignosulfonates from barley straw, and to determine if the optimal value found by the ANN model can be obtained with a low cost.

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AUTHORS BIOGRAPHY

Maria Guadalupe Serna-Diaz. She received the M.S. degree in Biotechnology from the Polytechnic University of Pachuca, in Pachuca de Soto, Hidalgo, Mexico, in 2011. Currently, she is a PhD student of the Polytechnic University of Pachuca, Pachuca de Soto, Hidalgo, Mexico.

Joselito Medina-Marin. He received the M.S. and Ph.D. degrees in electrical engineering from the Research and Advanced Studies Centre of the National Polytechnic Institute in Mexico, in 2002 and 2005, respectively. Currently, he is a Professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State in Pachuca, Hidalgo, México. His current research interests include Petri net theory and its applications, active databases, simulation, and programming languages.

Ainhoa Arana-Cuena. She received the Ph.D. degree in Molecular Biology from the Autonomous University of Madrid in Spain, in 2002, She is working as a full time professor in the Polytechnique University of Pachuca, in Hidalgo State, México. Her research interest is the applications of agricultural residuals.

Juan Carlos Seck-Tuoh-Mora. He received the M.S. and Ph.D. degrees in electrical engineering (option: Computing) from the Research and Advanced Studies Centre of the National Polytechnic Institute in Mexico, in 1999 and 2002, respectively. Currently, he is a Professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State in Pachuca, Hidalgo, México. His current research interests include cellular automata theory and its applications, evolutionary computing and simulation.

Alejandro Jurado-Tellez. He received the M.S. degree in Biotechnology from the Autonomous Metropolitan University, in México City, México in 1997, and the Ph.D. degree in Molecular Microbiology from the University of Alcalá in Spain, in 2002. He is working as a full time professor in the Polytechnique University of Pachuca, in Hidalgo State, México. His research interest is the applications of agricultural residuals.

Yuridia Mercado-Flores. She received the M.S. and Ph.D. degrees in Biotechnology from the National Polytechnic Institute in México, City, México, in 2002 and 2005, respectively. She is working as a full time professor in the Polytechnique University of Pachuca, in Hidalgo State, México. Her research interest is the applications of agricultural residuals.

Angélica Jiménez-González. She received the M.S. and Ph.D. degrees in Biotechnology from the Autonomous Metropolitan University, in México City, México, in 2003 and 2008, respectively. She is working as a full time professor in the Polytechnique University of Pachuca, in Hidalgo State, México. Her research interest is the applications of agricultural residuals.

Norberto Hernandez-Romero. He received the M.S. degree from Department of Electrical Engineering, Laguna Technological Institute at México, in 2001 and the Ph. D. from Autonomous University of Hidalgo State at México in 2009. Currently, he is a professor of the Advanced Research in Industrial Engineering Centre at the Autonomous University of Hidalgo State at Pachuca, Hidalgo, México. His current research interests include system identification, feedback control design, genetic algorithms, fuzzy logic, neural network and its applications

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