international journal of hydrogen energy XXX (2016) 1-19



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# Development of a mathematical methodology to investigate biohydrogen production from regional and national agricultural crop residues: A case study of Iran

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#### ARTICLE INFO

Article history: Received 30 July 2016 Received in revised form 29 September 2016 Accepted 3 October 2016 Available online xxx

#### Keywords:

Greenhouse gas emissions Agricultural residues Biohydrogen Social cost of carbon Monte Carlo simulation Time series

#### ABSTRACT

This study aims to construct a quantitative framework to assess biological production of hydrogen from agricultural residues in a country or region. The presented model is able to determine proper crops for biohydrogen production, its possible applications and use as well as environmental aspects. A multiplicative decomposition method was designed to forecast future production and Monte Carlo simulation was employed in the model to evaluate the risk of estimations.

From 2013 to 2050, the hydrogen production capacity could increase from 53.59 to 164.41 kilotonnes (kt) in Iran. The highest contribution to biohydrogen production (52.1% in 2013 and 73.3% in 2050) belongs to cereal crops including wheat, barley, rice and corn and the share of horticultural products including apples, grapes and dates is the lowest (2.7% in 2013 and 2.2% in 2050). For possible variations in the quantity of collectable residue and biohydrogen yield, the production may change in the range of 40.16% and 209.48% of the base value in 2013 and 41.64% and 233.18% of that in 2050. Ammonia production as nitrogen fertilizer and the area could be cultivated by that for each crop were calculated. The amount of natural gas saving and reduction in greenhouse gas (GHG) emissions using biohydrogen were discussed. Development of hydrogen fuel cell vehicles and their impacts on the environment and consequent social costs as well as the quantity of gasoline would be saved were estimated by 2050.

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#### Introduction

Opening the door to modern technologies based on harnessing biomass energy as the third largest primary source of energy in the world [1] has led to a promising perspective to tackle environmental issues and to supply global energy demand. Agricultural residues as one of the major sources of biomass have a heating value of about 12.56  $\times$  10<sup>6</sup> kJ t<sup>-1</sup> (equivalent to approximately 50% and 33% of that of coal and

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#### international journal of hydrogen energy XXX (2016) $1\!-\!\!19$

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# Nomenclature

А	area harvested, ha
а	the lowest value parameter of cumulative
	probability function
A <sub>CH3OF</sub>	quantity of methanol from biohydrogen, t
$A_{H_2}$	potential amount of produced biohydrogen, kg
$A_{H_2,T}$	total potential amount of produced biohydrogen,
	kg
$A_{NH_3}$	quantity of ammonia from biohydrogen, t
b	the most likely value parameter of cumulative
	probability function
с	the highest value parameter of cumulative
	probability function
CA	cultivable area by ammonia fertilizer (thousand
	ha)
Ст	annual production of crop. t
DS,	deseasonalized series
Fc	field cover factor, t ha <sup>-1</sup>
F <sub>CR</sub>	fraction of collectable residue
FE <sub>CV</sub>	average fuel economy of conventional vehicles,
	mile l <sup>-1</sup>
FGHG	amount of GHG emissions by process or end-use
GIIG	vehicles, kg CO <sub>2</sub> eq
$F_{H_2}$	annually required hydrogen for fueling hydrogen
2	fuel cell vehicles, kg
FEHECY	average fuel economy of hydrogen fuel cell
	vehicles, mile $kg^{-1}H_2$
FSCC	total social cost of carbon, \$
Ft	forecast in year, t
$h_h$	vield of hydrolysis of biopolymers to hexoses
hn	yield of hydrolysis of biopolymers to pentoses
I <sub>t</sub>	irregular component in year t
l <sub>h</sub>	loss of hexoses during operation
l <sub>n</sub>	loss of pentoses during operation
Ń	seasonal length
MMA <sub>t</sub>	M-step Moving Average
MI	average annual passenger car mileage, mile
	vehicle <sup>-1</sup>
$N_m$	number of matching seasonal factors
N <sub>PC</sub>	total passengers cars
NR	crop nitrogen requirement rate, kg N ha <sup>-1</sup>
Ns	time-series length
Р	cumulative probability
R <sup>2</sup>	coefficient of determination
r	portion of total required hydrogen fuel supplied by
	biohydrogen, %

r <sub>c</sub>	cellulose recovery after pretreatment
r <sub>h</sub>	hemicellulose recovery after pretreatment
R <sub>C</sub>	annual collectable quantity of residue, t
R <sub>M</sub>	maximum available residue, t
RPR	residue to product ratio
R <sub>T</sub>	annual production of residue, t
SCC	social cost of carbon, $t^{-1} CO_2 eq$
S <sub>CF</sub>	quantity of conventional fuel saved using
	hydrogen fuel cell vehicles, l
$S_{CH_4}$	amount of natural gas could be saved using the
	total biohydrogen, kg
SFt	seasonal factor in year, t
SI	seasonal index
SS <sub>R</sub>	residual sum of squares
SST	total sum of squares
St	seasonal component in year t
t	time, year
to	first year in time-series data
t <sub>f</sub>	last year in time-series data
Tt	trend component in year, t
WTW <sub>CF,m</sub>	<sub>ii</sub> average well-to-wheel GHG emissions factor of
	conventional vehicles, kg ${ m CO}_2$ eq mile $^{-1}$
$WTW_{H_2}$	average well-to-wheel GHG emissions factor of
	biohydrogen production, kg $CO_2$ eq kg <sup>-1</sup> H <sub>2</sub>
WTW <sub>H2,mi</sub>	average well-to-wheel GHG emissions factor of
	hydrogen fuel cell vehicles, kg CO $_2$ eq mile $^{-1}$
x <sub>c</sub>	mass fraction of cellulose in native residue
x <sub>h</sub>	mass fraction of hemicellulose in native residue
Уh	conversion yield of hexoses to biohydrogen
Ур	conversion yield of pentoses to biohydrogen
Y <sub>C</sub>	crop yield, t ha <sup>-1</sup>
Y <sub>CH₃OH</sub>	amount of hydrogen required for each tonne of
	methanol, kg $H_2$ t <sup>-1</sup> CH <sub>3</sub> OH
$Y_{CH_4/H_2}$	methane consumption per hydrogen production
	in a steam reforming process, kg $CH_4$ kg <sup>-1</sup> H <sub>2</sub>
$Y_{H_2}$	biohydrogen yield from crop residue, kg $t^{-1}$
	residue
$Y_{NH_3}$	amount of hydrogen required for each tonne of
	ammonia, kg $H_2 t^{-1} NH_3$
Y <sub>t</sub>	time-series data
α	contribution of hydrogen fuel cell vehicles to
	passenger car fleet, %
$\Delta_{GHG}$	reduction in GHG emissions, kg CO <sub>2</sub> eq
$\Delta_{ m SCC}$	reduction in social costs of carbon, \$

diesel, respectively) and a fuel value of  $1.86 \times 10^6$  kJ t<sup>-1</sup> (equivalent to approximately  $6.28 \times 10^6$  kJ bbl<sup>-1</sup> of that of diesel) [2]. In 2011, it was estimated that 11 billion tonnes of agricultural biomass were produced in around the world [3]. Geographical distributions of crop residues are more scattered in comparison to fossil reserves accumulated in limited regions of the world [4]. Owing to the limited amount of fossil fuels, being non-renewable, and greenhouse gases (GHG) emissions, extensive efforts are underway to exploit and

manage biomass energy in many different countries. In the United States from 2000 to 2015, the production of this energy increased about 61% and in 2015, it accounted for 46.56% of total renewable energy and 5.64% of the total US primary energy production [5]. From 2004 to 2014, the biofuels production was increased from 2035 to 11,683 million tonnes of oil equivalent (Mtoe) in Europe and Eurasia, 6488 to 31 252 Mtoe in North America, 7311 to 20,294 Mtoe in South and Center America and, overall, 16,445 to 70,792 in the world [6]. In

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