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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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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 $12.56 \times 10^6 \text{ kJ t}^{-1}$ (equivalent to approximately 50% and 33% of that of coal and

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Nomenclature			
A	area harvested, ha	r_c	cellulose recovery after pretreatment
a	the lowest value parameter of cumulative probability function	r_h	hemicellulose recovery after pretreatment
A_{CH_3OH}	quantity of methanol from biohydrogen, t	R_C	annual collectable quantity of residue, t
A_{H_2}	potential amount of produced biohydrogen, kg	R_M	maximum available residue, t
$A_{H_2,T}$	total potential amount of produced biohydrogen, kg	RPR	residue to product ratio
A_{NH_3}	quantity of ammonia from biohydrogen, t	R_T	annual production of residue, t
b	the most likely value parameter of cumulative probability function	SCC	social cost of carbon, \$ t ⁻¹ CO ₂ eq
c	the highest value parameter of cumulative probability function	SC_F	quantity of conventional fuel saved using hydrogen fuel cell vehicles, l
CA	cultivable area by ammonia fertilizer (thousand ha)	SC_{CH_4}	amount of natural gas could be saved using the total biohydrogen, kg
C_T	annual production of crop, t	SF_t	seasonal factor in year, t
DS_t	deseasonalized series	SI	seasonal index
F_C	field cover factor, t ha ⁻¹	SS_R	residual sum of squares
F_{CR}	fraction of collectable residue	SS_T	total sum of squares
FE_{CV}	average fuel economy of conventional vehicles, mile l ⁻¹	S_t	seasonal component in year t
F_{GHG}	amount of GHG emissions by process or end-use vehicles, kg CO ₂ eq	t	time, year
F_{H_2}	annually required hydrogen for fueling hydrogen fuel cell vehicles, kg	t_0	first year in time-series data
FE_{HFCV}	average fuel economy of hydrogen fuel cell vehicles, mile kg ⁻¹ H ₂	t_f	last year in time-series data
F_{SCC}	total social cost of carbon, \$	T_t	trend component in year, t
F_t	forecast in year, t	$WTW_{CF,mi}$	average well-to-wheel GHG emissions factor of conventional vehicles, kg CO ₂ eq mile ⁻¹
h_h	yield of hydrolysis of biopolymers to hexoses	WTW_{H_2}	average well-to-wheel GHG emissions factor of biohydrogen production, kg CO ₂ eq kg ⁻¹ H ₂
h_p	yield of hydrolysis of biopolymers to pentoses	$WTW_{H_2,mi}$	average well-to-wheel GHG emissions factor of hydrogen fuel cell vehicles, kg CO ₂ eq mile ⁻¹
I_t	irregular component in year t	x_c	mass fraction of cellulose in native residue
l_h	loss of hexoses during operation	x_h	mass fraction of hemicellulose in native residue
l_p	loss of pentoses during operation	y_h	conversion yield of hexoses to biohydrogen
M	seasonal length	y_p	conversion yield of pentoses to biohydrogen
MMA_t	M-step Moving Average	Y_C	crop yield, t ha ⁻¹
MI	average annual passenger car mileage, mile vehicle ⁻¹	Y_{CH_3OH}	amount of hydrogen required for each tonne of methanol, kg H ₂ t ⁻¹ CH ₃ OH
N_m	number of matching seasonal factors	Y_{CH_4/H_2}	methane consumption per hydrogen production in a steam reforming process, kg CH ₄ kg ⁻¹ H ₂
N_{PC}	total passengers cars	Y_{H_2}	biohydrogen yield from crop residue, kg t ⁻¹ residue
NR	crop nitrogen requirement rate, kg N ha ⁻¹	Y_{NH_3}	amount of hydrogen required for each tonne of ammonia, kg H ₂ t ⁻¹ NH ₃
N_S	time-series length	Y_t	time-series data
P	cumulative probability	α	contribution of hydrogen fuel cell vehicles to passenger car fleet, %
R^2	coefficient of determination	Δ_{GHG}	reduction in GHG emissions, kg CO ₂ eq
r	portion of total required hydrogen fuel supplied by biohydrogen, %	Δ_{SCC}	reduction in social costs of carbon, \$

diesel, respectively) and a fuel value of 1.86×10^6 kJ t⁻¹ (equivalent to approximately 6.28×10^6 kJ bbl⁻¹ 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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