# PRELIMINARY EXPERIMENTAL RESULTS OF IGFC OPERATION USING HARDWARE SIMULATION

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## ABSTRACT

A newly developed Integrated Gasification Fuel Cell (IGFC) hybrid system concept has been tested using the Hybrid Performance (Hyper) project hardware-based simulation facility at the U.S. Department of Energy, National Energy Technology Laboratory. The cathode-loop hardware facility, previously connected to the real-time fuel cell model, was expanded by the inclusion of a real-time model of a gasifier of solid fuels, in this case biomass fuel. The fuel cell is operated at the compressor delivery pressure, and it is fuelled by an updraft atmospheric gasifier, through the syngas conditioning train for tar removal and syngas compression. The system was brought to steady-state; then, several perturbations in open loop (variable speed) and closed loop (constant speed) were performed in order to characterize the IGFC behavior. Experiments have shown the feasibility of relatively fast control of the plant as well as a possible mitigation strategy to reduce the thermal stress on the fuel cell as a consequence of load variation and change in gasifier operating conditions. Results also provided an insight into the different features of variable vs constant speed operation of the gas turbine section.

## INTRODUCTION

Hybrid fuel cell turbine power systems (FC/GT) represent an opportunity to almost double the efficiency of standard pulverized coal power generation technology and reduce harmful emissions associated with power generation by 50%[1][2]. To reach this level of efficiency, the complexities of the highly coupled FC/GT cycle have been addressed and are currently being resolved at the U.S. Department of Energy, National Energy Technology Laboratory (NETL) for all stages of operation, from startup to shutdown. The Hybrid Performance (Hyper) project at NETL makes use of hardware simulation of a 200kW to 700kW solid oxide fuel cell (SOFC)

system coupled to a 120kW turbine [3]. This is accomplished through a Hardware-in-the-Loop Simulation (HILS) approach to study direct-fired, recuperated hybrid systems [4].

One inherent complexity of the FC/GT hybrid system comes from wide discrepancies in the individual component response times. It is well known that the mismatch between fuel cell and balance of plant time constants make the control task arduous for all operating regimes.

In the case of the Hyper facility, pressure vessels and a natural gas burner driven by real time models are used to simulate the fuel cell and gasifier in the system. The hardware simulating the fuel cell is then integrated with turbomachinery, a generator, a continuously variable load bank, exhaust gas recuperators, and the associated valves needed to control the system airflow. This approach takes advantage of the flexibility associated with numerical models and the fidelity associated with hardware.

Since the fuel cell is the most expensive component in an IGFC, the use of robust hardware in its simulation allows for the evaluation of complex control strategies and dynamic performance during transient operation without significant financial risk.

A diagram of the Hyper facility with corresponding numerical components used in the present work is shown in Figure 1. A direct fired, recuperated cycle operating on coal/biomass syngas was chosen for study based on its potential for high efficiency.

The major hardware components of the Hyper facility are shown with the integrated fuel cell model in Figure 2. The combination of the cathode air plenum (V-301), the post combustor mixing plenum (V-304), and the system burner (V-302) are used to simulate the dynamic response of the fuel cell in the system hardware. A distributed fuel cell model is used for the current study [5].



Figure 1 – Hyper facility with corresponding virtual components



Figure 2 – Simplified Flow Diagram for the Hybrid Performance Simulation Facility at NETL

#### **EXPERIMENTAL FACILITY**

#### Hardware

The Hyper simulation facility uses a combination of hardware and real time dynamic models to simulate a solid oxide fuel cell gas turbine hybrid system, as shown in Figure 2. The process has been described in detail elsewhere, and so the following description has been abbreviated [3][6].

## Gas Turbine (C-100, T-101, G-102)

A 120kW Garrett Series 85 auxiliary power unit (APU) is used for the turbine and compressor system, and consists of single shaft, direct coupled turbine (T-101) operating at a nominal 40,500rpm, a two-stage radial compressor (C-100) and gear driven synchronous (400Hz) generator (G-102). The electrical generator is loaded by an isolated 120kW resistor bank (E-105). The compressor is designed to deliver approximately 2 kg/s at a pressure ratio of about four. The compressor discharge temperature is typically 475K for an inlet temperature of 298K. The combustor and original fuel system was removed. The turbine runs only on heat provided by the fuel cell simulator (V-302), upstream of the post combustor (V-304).

## Heat Exchangers (E-300 and E-305)

The facility includes two counter flow primary surface recuperators (E-300 and E-305) in parallel with a nominal effectiveness of 89% to preheat the air fed to V-301, which represents the fuel cell cathodic chamber and oxidant manifolding volume [7].

### Pressure Vessels (V-301 and V-304)

Pressure vessels are used to provide the representative fuel cell air manifold and cathode volume (V-301), and the post combustion volume (V-304) of the fuel cell system.

# Fuel Cell Simulator (V-302)

The thermal characteristic of the effluent exiting the post combustor of an SOFC system is simulated in hardware using a natural gas burner with an air-cooled diffusion flame.

## Cold-Air Bypass (FV-170)

The cold-air bypass valve is used to bypass air from the compressor directly into the turbine inlet through the post combustor volume.

## Hot-Air Bypass (FV-380)

The hot-air bypass valve is used to bypass air from the recuperators exit directly into the turbine inlet through the post combustor volume.

# Bleed-Air (FV-162)

The bleed valve is used to discharge cold compressed air into the atmosphere. It is very effective in augmenting compressor surge margin, but it detrimentally affects system efficiency.

#### Instrumentation

A detailed discussion of the sensors used for collecting process data is discussed in previous work [6]. A brief description of key instrumentation is included in the following discussion, and refers to Figure 2 where tag numbers are used to identify the sensors.

#### Rotational Speed Measurement (ST-502)

Rotational speed is measured by an optical sensor (ST-502) which picks up laser light reflected from a rotating target on the end of the generator shaft and transmits the pulse train to the frequency input of the control system.

# Compressor Inlet Flow (FE-110)

Compressor inlet flow is measured using an annubar flow element (FE-110), which provides a mechanical average of the difference between stagnation pressure and static pressure in the inlet pipe to determine flow. Compressor inlet temperature (TE-112) and pressure (PT-116) reflect ambient conditions in the facility test cell during operation, and are used for calculating referred or corrected air flow and compressor pressure ratio.

## Bypass Flow (FE-162)

Compressor bleed and cold air bypass airflows are measured using an annubar flow meter (FE-162) similar to FE-110. Compressor discharge temperature (TE-147) and pressure (PT-151) are measured in the compressor plenum, just after the diffuser and before the airflow has circulated around the turbine scroll.

## Fuel Cell Simulator Flow (FE-380)

Primary airflow through the fuel cell simulator is measured at the entrance of V-301 using an annubar flow meter (FE-380) similar to FE-110. The combined temperature of the mixed streams from the heat exchangers (TE-326) is measured just up stream of the hot-air bypass valve, FV-380. Pressure is measured inside the air plenum of the fuel cell simulator (V-301) using PT-305.

## Fuel Cell Model

Previously, NETL developed a lumped parameter real-time fuel cell model that was successfully coupled with the hybrid arrangement using hardware based simulation [8]. For this study, a one-dimensional thermal and electrochemical model of a planar SOFC using finite discretization techniques was used to run the Hyper facility in real time. The preliminary spatiotemporal model provides the user the ability to observe and capture local, internal tranport phenomena of an operating fuel cell with variable levels of spatial resolution and during transient modes. For the sake of this study, the model generates gas and solid fuel cell temperature profiles in spatial and temporal regimes. A more comprehensive and higher fidelity version of the model was subsequently developed [9].

Each individual cell is constructed of an anode, electrolyte, cathode and two, 441SS interconnects, one on either side of the positive-electrolyte-negative (PEN) structure. Interconnects represent the bulk of the fuel cell solid mass. The fuel cell stack is comprised of 2300 cells with an approximate 350kW rating. Curve fits of the thermophysical data were used to incorporate the temperature dependence of these properties in the model.

Computationally, a single 20cm x 20cm cell is modeled with the inlet and outlet flow rates scaled by a factor of 2300. Each cell was discretized into evenly spaced volumes spaced at 10mm intervals and arranged parallel to the direction of reactant flow, with node 1 representing the inlet volume and node "N" representing the outlet volume. At each time step, the model updates all discretized values.

The cell operating voltage is calculated according to the Nernst potential, with additional consideration of the electrochemical losses produced by activation, ohmic (including contact resistance), and concentration phenomema [5]. The model allows for a rapid real-time implementation via streamlined, yet sufficient, calculations.

Normally, the model is used to dynamically calculate the thermal effluent of a stack based upon measured Hyper flow conditions and user set points, and assumes the use of syngas as fuel. The cathode inlet airflow and pressure are measured by FE-380 and PT-305, respectively. The cathode inlet airflow

temperature is assumed to pass through a high-temperature heat exchanger, which elevates its temperature (experimentally measured at TE-326) by a pre-determined  $\Delta T$  (usually in the 200-300K range): the same  $\Delta T$  is applied to the fuel cell effluents, from which the heat is assumed to be extracted. This approximation does not account for differing heat capacity rates between the hot and cold streams in a virtual heat exchanger; but it's an appropriate simplification given the overarching scope. The experimental data is used as input to the fuel cell model along with user specified fuel and electric load applied to the fuel cell; as shown in Figures 1-2. In this case fuel flow and composition are provided by the gasifier model through the syngas conditioning unit.

## FACILITY UPGRADE: THE GASIFIER MODEL

The collaboration with the Thermochemical Power Group of the University of Genoa, Italy, resulted in the implementation of a gasifier model for real time application into the Hyper facility. The gasifier is meant to provide syngas to the fuel cell, thus realizing a novel "virtual" Integrated Gasification Fuel Cell (IGFC). The integrated facility with the gasifier connected to the fuel cell and gas turbine hardware was successfully tested for the first time in July 2010. The modeling work targeted the development of a generic "Thermal Network Library", based in Matlab-Simulink, and relying mainly on Embedded Matlab Functions originally developed for this purpose. Such a library is composed of the following three main components:

- 1. <u>Solid Domain</u>, simulating a 2-D solid matrix with internal conductive heat transfer.
- 2. <u>Fluid Domain</u>, simulating a quasi 2-D reacting flow of solid/liquid/gas.
- 3. <u>Heat Linker</u>, defining the heat exchange relationships between the boundaries of solid and fluid domains.

Such components use a finite-difference formulation of the thermal problem, which is resolved with an implicit time integration scheme.

In the following, only the "Fluid Domain" component is described in details, as it is the most significant one for the case study presented (the other two are only used to represent the thermal loss to the ambient, in this specific case).

## Numerical scheme

The finite difference mathematical scheme in Figure 3 has been developed and implemented, with the division into two main parts: the solid phase (bottom) and the vapor phase (top). On the x axis, the domain is discretised into xN cells, with, in general, variable space steps ( $\Delta x_i$ ).

The internal surfaces on the vertical plane, i.e. the section of mass transport  $(Sy_j)$ , are derived by linear interpolation from the boundary surfaces, provided via input by the user.

The interface surface between solid and vapor phases is subdivided proportionally to the space steps along the x axis  $(Sx_i)$ .

The external heat sources are input to the model: they are to be calculated and provided by the Heat Linker component. The resulting numerical approach is quasi 2-D, as it considers fully 1-D discretisation for both the solid and vapor phases. The thermal nodes of each cell is centered at the cell face, in order to allow a easier implementation of mass transport along the x axis. The vapor flow direction can be chosen to be co-flow or counter-flow with the solid phase.

The generic time-dependent energy equation for the generic ith cell is expressed by (1),

$$\frac{\partial (M_{i,j}c_{v,i,j}T_{i,j})}{\partial t} = \sum_{in} mf \cdot c_{p} \cdot T - \sum_{out} mf \cdot c_{p} \cdot T \pm q_{exch\,i} + qs_{i,j} + qreaction_{i,j}$$
(1)
where:

- M is the mass of the infinitesimal cell [kg];
- c<sub>p</sub> is the specific heat at constant pressure [J/kg K];
- $c_v$  is the specific heat at constant volume [J/kg K];
- T is the temperature [K];
- "q" are heat fluxes (qs are heat sources, as illustrated in Figure 3) [W];
- "mf" are the mass flows [kg/s];
- "in", "out", "react" subscripts refer to cell inlet, cell outlet, reactions occurring in the cell.

The energy balance equation can be written as shown in (2)-(4), for the case of co-flow configuration.

$$q_{exch i} = h_{conv i} Sx_i (T_{i+I,I} - T_{i+I,2})$$

$$\frac{\partial (M_{i-I,I} c_{v i-I,I} T_{i,I})}{\partial t} =$$

$$(mf \cdot c_p \cdot T)_{i-I,I} - (mf \cdot c_p \cdot T)_{i,I} - (\Delta m f_{i-I} \cdot c_{pi,I} \cdot T_{i,I}) +$$

$$-q_{exch i-I} + qs_{bottom i-I} + \sum_{pyrolysis, gasification} \Delta m f_{i-I} \cdot \Delta h$$

$$for j=1 (solid phase) and i>1$$

$$(2)$$

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$$\frac{\partial \left(M_{i-l,2}c_{v,i-l,2}T_{i,2}\right)}{\partial t} = (mf \cdot c_{p} \cdot T)_{i-l,2} - (mf \cdot c_{p} \cdot T)_{i,2} + (\Delta mf_{i-l} \cdot c_{p,i,l} \cdot T_{i,l}) + + q_{exch \ i-l} + qs_{top \ i-l} + q_{Gibbs \ i-l}$$
(4)  
for i=2 (vapor phase) and i>1

where

- "Δh" is the heat of reaction due to pyrolysis and gasification reactions [J/kg];
- "q<sub>Gibbs</sub>" is the heat of reaction due to equilibrium calculation at the reactor outlet (total heat is subdivided among the cells proportionally to vapor mass flow) [W];



Figure 3 – Fluid domain: transient model finite difference scheme

In case the flow configuration is counter-flow (see Figure 3), the (2)-(4) modify into (5)-(7). The energy equation is solved implicitly in the temperatures, assuming constant (within the integration time step) all coefficients and heat sources, including heat of reaction: thus, the energy equation reduces to a system of linear equations where the temperatures T are unknown. In such a linear representation of the thermal problem, the unknowns are the temperatures at the new time constant. The square matrix of coefficients have dimensions equal to  $(xN \cdot 2) X (xN \cdot 2)$ , where "2" indicates the two solid and vapor phases – the solid and vapor inlet temperatures are known as they are boundary conditions. Overall, the linear system in temperatures can be resolved in an implicit away, ensuring stability of the time-dependent solution.

$$q_{exch i} = h_{conv i} Sx_i (T_{i+I,I} - T_{i,2})$$

$$\frac{\partial (M_{i-I,I}c_{v i-I,I}T_{i,I})}{\partial t} =$$

$$(mf \cdot c_p \cdot T)_{i-I,I} - (mf \cdot c_p \cdot T)_{i,I} - (\Delta mf_{i-I} \cdot c_{pi,I} \cdot T_{i,I}) +$$

$$-q_{exch i-I} + qs_{bottom i-I} + \sum_{pyrolysis, gasification} \Delta mf_{i-I} \cdot \Delta h$$
for j=1 (solid phase) and i>1
$$(5)$$

$$\frac{\partial \left(M_{i,2}c_{v,i,2}T_{i,2}\right)}{\partial t} =$$

$$\left(mf \cdot c_{p} \cdot T\right)_{i+1,2} - \left(mf \cdot c_{p} \cdot T\right)_{i,2} + \left(\Delta mf_{i} \cdot c_{pi+1,1} \cdot T_{i+1,1}\right) + q_{exch\ i} + q_{Sibbs\ i}$$

$$(7)$$

for j=2 (vapor phase) and i<xN+1

#### **Cascaded reactions**

Physical and chemical reactions have been modeled using a kinetic cascaded approach. In particular, it has been assumed that:

- Drying and pyrolysis occur at very different temperatures, so that there is no interference between the processes.
- Once pyrolysis has occurred, the remaining char is assumed to undergo gasification reactions. In particular, the most relevant ones are, in order of kinetic speed, O<sub>2</sub> gasification/combustion, H<sub>2</sub>O gasification, CO<sub>2</sub> gasification. The hydro-gasification reaction, i.e. H<sub>2</sub> gasification, has not been considered, as it tends to be significantly slower than the previous ones [10].
- Char gasification is considered to happen in a cascade: first O<sub>2</sub> gasification/combustion occurs, due to the high reactivity of O<sub>2</sub>. The char left by O<sub>2</sub> reactions is considered to be available for H<sub>2</sub>O and CO<sub>2</sub> gasification, which follows.

• The remaining O<sub>2</sub> is finally considered available for CH<sub>4</sub>, H<sub>2</sub> and CO oxidation kinetics, which are executed in series.

#### Heterogeneous reactions: drying and pyrolysis

The pyrolysis model is taken from [11]. Even if the macroparticle model has been reproduced, it was decided to implement the micro-particle model only, in order to allow real-time simulation. In fact, the macro-particle model would require too much computational effort. In this respect, since the micro-particle model does not include particle internal heat transfer and diffusion resistances, apparent intrinsic pyrolysis kinetics should be employed (i.e.: kinetics obtained from realsize particles).

The model requires as input the mass fractions of biomass in terms of humidity, ash, cellulose, hemicellulose and lignin. Examples of cellulose, hemicellulose and lignin contents are reported in Table 1.

Table 1 – Dry mineral material free composition of representative biomasses [11]. Note: ashes and extractives have been included in the hemicellulose fraction, as it improved numerical results, according to [11]

	Cellulose	Hemicellulose	Lignin
Bagasse	0.36	0.47	0.17
Beech	0.48	0.28	0.24
Cherry	0.42	0.34	0.24
Maple	0.40	0.38	0.22
Oak	0.35	0.40	0.25
Olive husk	0.22	0.33	0.45
Pine	0.50	0.27	0.23
Poplar	0.48	0.30	0.22

The generic reaction scheme is reported in Figure 4.



Figure 4 – Generic reaction scheme used to model cellulose, hemicellulose and lignin pyrolysis (blue and black arrows). Red arrows regard char gasification. The generic rate  $K_j$  is expressed by an Arrenius-type equation, conveyed in (11). All kinetic parameters and heats of reaction have been derived from [11].

$$K_j = A_j e^{-\frac{E_j}{\Re T}} \tag{11}$$

Additionally, fictitious evaporation kinetics have been added, as shown in Figure 4. The related frequency constant A and activation energy E are:

where the activation energy is corrected by water saturation temperature (which is dependent on reactor total pressure) to ensure water evaporation at the correct temperature level.

The pyrolysis model does not need the ultimate composition of biomass, i.e. C, O, H, S, N contents. So, accordingly, tar and char compositions are not calculated. There are two options for the pyrolysis gas composition (primary and secondary gases are considered mixed together):

- 1. <u>Fixed composition</u>. Pyrolysis gas composition is provided by the user as an assumption: as a result, the overall mass balance is respected, while the single species mass balance is disregarded. This approach is recommended for exploring new operating points for the first time.
- 2. <u>Mass balanced</u>. The composition is derived from the mass balance of elementary species (CHO). Assumptions:  $H_2O$  and  $CH_4$  molar contents of pyrolysis gas; char is pure carbon "C"; all the input biomass, apart from char, has been converted to pyrolysis gas. When tar is present in the output gas, the mass balance can be considered approximated only.

#### Heterogeneous reactions: O2 char gasification

 $O_2$  gasification/combustion has been modeled according to [12]. The model was developed for coal char samples, but it was assumed the same for biomass char. In fact,  $O_2$  reactivity is already quite high, so the highest reactivity of biomass char would not change significantly the relationship between this fast reaction and the much slower  $H_2O$  and  $CO_2$  gasification reactions.

Char consumption within a system containing low levels of moisture primarily proceeds by two gas-solid reactions: an exothermic C-O<sub>2</sub> reaction seen in (12) and (2) an endothermic C-CO<sub>2</sub> reaction: the latter has been considered together with  $H_2O$  gasification, and described later. The overall exothermic reaction is shown in (12),

$$\frac{2(\eta+1)}{(\eta+2)}C+O_2 \xrightarrow{2\eta} (\eta+2)CO+\frac{2}{(\eta+2)}CO_2$$
(12)

where  $\eta$  is the primary CO/CO2 molar ratio.

The primary  $CO/CO_2$  product ratio can be correlated by the Arrhenius relationship of (13).

$$\eta = 70e^{-3070/T}$$
 (13)

The intrinsic rate followed can be expressed by (14),

$$r_{O2} = \frac{2(\eta+1)}{(\eta+2)} \cdot M_{char} \cdot Sa \cdot C_{O2} \cdot kr \cdot T \cdot e^{-21578/T}$$
(14)

where

$$r_{O2}$$
 rate of char consumption due to  $O_2$   
gasification/combustion [kg<sub>char</sub>/kg<sub>char</sub> s];

 $C_{O2} = P_{O2} / (\mathcal{R}^*T)$  is the O<sub>2</sub> concentration [kmol/m<sup>3</sup>];

- Mchar =12 [kg/kmol], molecular weight of char, which is considered pure C;
- kr =10.46 [m/s], rate constant for reaction;

Sa =600.e+03  $[m^2/kg_{char}]$  active surface;

Sa value was derived considering the rate expression provided by [12] for char CO<sub>2</sub> gasification, and comparing the obtained rates with [13] and [14]. While a value of about 200.e+03 would provide rates consistent with Dutta et al. 1977 [14], this higher value provides results that are aligned with Gobel 2001 [13]: however, Dutta [14] studied coal char gasification while Gobel [13] considered biomass char gasification. Thus the highest value is retained and can be justified by considering the higher reactivity of biomass char respect to coal char.

The heats of reaction have been considered constant and reported in (15) for partial and complete combustion: water is considered at the gaseous state; reference enthalpies of formation are derived from [12], where standard conditions are  $25^{\circ}$ C and 1 atm.

$$C+1/2 O_2 \rightarrow CO \qquad \Delta h = -110.5 \cdot 10^3 \text{ kJ/kmol}$$

$$C+O_2 \rightarrow CO_2 \qquad \Delta h = -393.4 \cdot 10^3 \text{ kJ/kmol}$$
(15)

#### Heterogeneous reactions: H<sub>2</sub>O and CO<sub>2</sub> char gasification

 $H_2O$  and  $CO_2$  gasification reactions have been modeled in accordance to [13]. Overall reactions and heats of reaction (considered constant) are reported in (16).

C+H2O
$$\rightarrow$$
CO + H2  $\Delta h = +131.0 \cdot 10^{3} \text{ kJ/kmol}$   
C+CO2 $\rightarrow$ 2CO  $\Delta h = +172.4 \cdot 10^{3} \text{ kJ/kmol}$  (16)

The reactivity of a solid fuel is commonly described as a function of the fractional conversion or burn-off X,

$$r = -\frac{1}{m}\frac{dm}{dt} = \frac{1}{1-X}\frac{dX}{dt}$$
 with  $X = \frac{m_0 - m}{m_0}$  (17)

where "m" is the mass of organic material during the conversion.

One common approach to model r is to split its expression into two terms (18): the first relating to the chemical kinetic  $r_c$ (dependent upon temperature and chemical composition and/or pressures) and the second depending on X, providing the socalled "structural profile" f(X): f(X) is usually defined with reference to the 50% burn-off case, so that f(0.5) = 1.

$$r = r_c \cdot f(X) \tag{18}$$

The following expression (19) based on Langmuir-Hishelwood kinetics is used to describe the kinetic parameters in the gasification of mixtures  $H_2O/CO_2/H_2/CO$ , so that the inhibiting effects of  $H_2$  and CO are effectively taken into account.

$$r = \frac{k_{1,fw} \cdot P_{H2O} + k_{1,fc} \cdot P_{CO2}}{1 + \frac{k_{1,fw}}{k_3} \cdot P_{H2O} + \frac{k_{1,fc}}{k_3} \cdot P_{CO2} + \frac{k_{1,bw}}{k_3} \cdot P_{H2} + \frac{k_{1,bc}}{k_3} \cdot P_{CO}} \cdot f(X)$$
(19)

$$C_{f} + H_{2}O \xrightarrow[k_{1,fw}]{k_{1,fw}} C(O) + H_{2}$$

$$C(O) \xrightarrow{k_{3}} CO$$

 $C_{f} + CO_{2} \xrightarrow{k_{1,fc}} C(O) + CO$   $C(O) \xrightarrow{k_{3}} CO$ (20)

Such a kinetic scheme is referred to the 2-step Ergun and Reif reaction mechanism of carbon gasification with either  $H_2O$  or  $CO_2$  shown in (20). The generic rates k are expressed by Arrenius-type equations, such as (11). All kinetic parameters have been derived from Table 1 and 2 of [13].

#### Homogeneous reactions: CH<sub>4</sub>, H<sub>2</sub>, CO oxidation

 $CH_4$  partial oxidation,  $H_2$  and CO complete oxidation have been modeled according to [15]. This reference presented some inaccuracies in the coefficients reported for the kinetic mechanisms (Table 2 in [15]), so they have been checked and corrected in the following way:

- CH<sub>4</sub> partial oxidation global kinetic scheme has been taken from the original reference [16].
- H<sub>2</sub> complete oxidation global kinetic scheme has been taken from the original reference [16].
- CO complete oxidation global kinetic scheme was not published by Westbrook and Dryer in the cited reference [17]. So, it was preferred to derive such a scheme from [18], who quoted a more recent work from the same authors [19].

In the end, reaction kinetics have been implemented for the following three reactions:

 $\begin{array}{cc} K_{A} \\ CH4+1/2 \text{ } O2 \longrightarrow CO + 2H2 \\ K_{B} \\ H2 +1/2 \text{ } O2 \longrightarrow H2O \\ K_{C} \\ CO + 1/2 \text{ } O2 \longrightarrow CO2 \\ \end{array} \qquad \Delta h = -241.5 \cdot 10^{3} \text{ kJ/kmol} \qquad (22)$ 

The global generic kinetic rate expression is reported by (23), and related coefficients are summarized in Table 2.

$$K = A \cdot T^{n} e^{\frac{E}{\Re T}} \cdot C x^{a} C y^{b}$$
<sup>(23)</sup>

where

Κ	is the reaction rate [kmol/m <sup>3</sup> s]
А	is the pre-exponential factor [dimensions vary
	depending on n, a and b]
Т	is the temperature [K]
n	is the exponent of temperature
Е	is the activation energy [kJ/kmol]
$\mathcal{R}$	is universal gas constant [8.314 kJ/kmol K]
Cx, Cy	are concentration of gases x and y $[kmol/m^3]$

#### Homogeneous chemical reactions: Gibbs reactor

Homogeneous chemical reactions are lumped at the exit of the gasifier, taking place in the so-called "Gibbs reactor", which brings the gas composition to equilibrium (without involving vapor tar) through minimization of Gibbs free energy of the output stream, at constant temperature. The resulting heat of reaction is then distributed along the vapor cells of the Fluid Domain, proportionally to the total vapor mass flow.

For this case-study, such a component has not been employed, as described later.

#### Phenomena not included in the model

The real-time application of the model constrained the developers to avoid the inclusion of some real effects that may occur in a gasifier. The main phenomena not represented at the moment are:

- <u>mass accumulation</u> => the level of solid is pre-defined, as well as the surface available for the vapor phase. Thus, start-up phenomena cannot be captured.
- <u>tar condensation</u> => tar is considered to be always in the vapor phase, together with the incondensable gases and steam.
- <u>diffusion and heat resistance</u> => diffusion and heat resistance within the solid particles is not considered (intrinsic apparent kinetics should be used), thus particle size has no influence on results.

#### **Model verification**

To verify the results of the Fluid Domain component, the following verifications have been performed successfully:

- Check the independence from space and time discretisation.
- Verification of the pyrolysis micro-particle model against original paper results.

 Table 2 – Kinetic parameters for the homogeneous gas reactions. Sample K values have been computed for 1000K and Cx=Cy=0.01 kmol/m<sup>3</sup>

	А	n	Е	Cx <sup>a</sup>	Cy <sup>b</sup>	Ref	sample K
K <sub>A</sub>	4.4 e+11	0	1.255 e+5	[CH4] <sup>1/2</sup>	$[O_2]^{5/4}$	[16]	38.71
K <sub>B</sub>	6.8 e+15	-1	1.6744 e+5	$[H2]^{1/4}$	[O2] <sup>3/2</sup>	[16]	3.855
K <sub>C</sub>	2.24 e+12	0	1.703 e+5	[CO]	[H2O]	[18]	0.2823

- Verification of the gasification model against literature data.
- Verification of mass and energy overall balances at regime.
- Verification of CHO species mass balance, in case of complete conversion of tar, at regime.
- Check the transient response against the existing TRANSEO model of a recuperator (comparison was made with the gas part of it, inhibiting all the chemical reactions on the solid phase) [20][21].
- Check against an ASPEN gasifier equilibrium model developed at NETL (results to be published soon).

As a future work, authors are currently addressing the design of targeted experiments at NETL facilities in order to collect enough time-dependent data to validate the model.

# CASE STUDY

The NETL facility was operated connected to the gasifier realtime model providing syngas to the syngas cleaning unit and then to the fuel cell model (see Figure 1).

The <u>syngas conditioning unit</u> is quite simple at this stage, as it only reduces water content to about 10% molar fraction, and it assumes to clean out all tars. In this case sulfur is not an issue as the input biomass is considered sulfur-free. As far as the dynamic response is concerned, no time delays are introduced.

In this case study, the gasifier model was representing a scaleddown version of the Danish Harboore atmospheric updraft gasifier, for which extensive operational data can be found in open literature. A recent publication reporting many details is [22]. The gasifier has an internal diameter of 1.2m and total height of 8m: the latter was oversized in order to ensure enough residence time for the input wet biomass to dry. The design load is about 2MWth. Biomass is fed from the top while preheated humid air is injected at the bottom. It was decided to start with this kind of "old-style" and somewhat inefficient gasifier because of its features in terms of robustness and stability of operation. In fact, the large amount of biomass stored in the reactor allows large steps in the oxidant flow without compromising too quickly the output gas quality and the thermal stability of the gasifier itself. In this simulation case, pyrolysis gas composition was assumed (fixed composition option mentioned before).

The starting operating point of the overall IGFC cycle is reported in Table 3. The gasifier was being operated at full load, while the system was run at relatively low utilization factor and low air flow through the fuel cell (i.e. almost half air flow bypassed or bled). A relatively inefficient operating point was motivated for being the first transient analysis performed on the IGFC cycle, then the priority was to have a robust and stable (rather than efficient) operating point around which to try some transients, avoiding compressor surge and reducing the fuel cell impact on the system dynamic response. Such a "safe margin" can be reduced in the future, after the dynamic response is better understood, thus starting from a more efficient initial operating condition.

Input biomass flow [kg/s] and LHV [kJ/kg] 0.21 9340 Input biomass humidity [mass%] 42% 34% 39% 25% Cellulose, Hemicellulose, Lignin, Ash contents [mass%] 2% Oxidant agent flow [kg/s] and temp.[K] 0.14 423.15 62% 16% 22% Oxidant agent comp. [mol% N2, O2, H2O] Output Gas mass% mol% 28.2 22.5  $N_2$  $O_2$ 0.0 0 H<sub>2</sub>O 36.6 45.2 CO 14.8 11.8  $CO_2$ 11.6 5.9 H2 1.0 11.4  $CH_4$ 1.4 1.9 6.5 Tar 1.4 Power In, Out w/tar, Out w/o tar [MWth] 1.96 1.53 1.11 Fuel Cell Syngas scaler (fuel fraction used in FC) 88% Total current [A] and av. density  $[A/cm^2]$ 200 0.5 0.77 0.94 Operating and av. Nernst voltages [V] DC electrical power [kW] 355 Fuel utilization 62% Cold syngas efficiency\* 36% Gas Turbine Ambient temp. [K] and pressure [bar] 306 0.969 Intake air and FC cathode air flows [kg/s] 2.1 1.3 Bleed air [%opening, estimated kg/s] 8% 0.1 Cold air bypass [%opening, estimated 40% 0.7 kg/s] Hot air bypass [%opening, estimated kg/s] 10% 0.01 Rotational speed [rpm] 40500 AC Electrical power [kW] 45 System Cold syngas thermal input\* [kW] 980 389 System AC power\* [kW] Cold syngas efficiency\* 40%

 Table 3 – Starting operating point of the IGFC plant

 Gasifier

\* considers only the fraction of syngas sent to the system, indicated by the syngas scaler. DC power is decreased by 3% because of inverter losses.

Figure 5 reports the initial profile of solid and vapor mass flows, which are in counter-flow, along the gasifier height: the non-fully smooth behavior is due to the number of nodes (10 in this case) to allow real-time execution. From right to left, the solid mass flow decreases first because of drying, then because of pyrolysis, finally because of gasification/combustion: ash and remaining char are discharged at the bottom. Vapor flow increases because of the air injection (happening between node 0 and 1) and of biomass reactions. Figure 6 illustrates the temperature profile calculated within the gasifier walls: it is clear that more than half of the height is used only for drying the biomass, before it gets into the pyrolysis-gasification zone. Before leaving the reactor from the bottom, ash and remaining char are quenched down by the injected oxidant agent, i.e. pre-heated humid air in this case. The refractory and insulation thicknesses are enough in order to bring the skin temperature down to about 373K at the bottom.



Figure 5 – Gasifier initial mass flow profile. Height: 0. is bottom, 8. is top.



Figure 6 – Gasifier wall initial temperature flow profile. Height: 0. is bottom, 8. is top. Thickness: 0.-0.01 is skin, 0.01-0.0500 is insulation, 0.05-0.25 is refractory.

Finally, Figure 7 shows the operating conditions of the fuel cell, along its 20 nodes of discretisation. The fuel cell is

operated at constant voltage (see Table 3), thus current density varies along the axis: at node 1 the current density is modest because of the lower temperature; at node 20 the current density is low because the Nernst voltage dropped significantly as a consequence of fuel utilization; thus, an internal peak in current density shows up just before the cell centerline, which is also where the temperature spatial gradient is the highest, as shown later in Figure 13.



Figure 7 – Fuel cell internal profiles. Node 1, on the left, is fuel and air inlet, Node 20, on the right, is fuel and air outlet (co-flow configuration).

From the steady-state point reported in Table 3, the system was perturbated as illustrated in Figure 8 (the approximate time instant is reported Table 4).

Tal	ble	4 –	Sys	tem	per	tur	bat	tions
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Gas turbine in open loop, i.e. variable speed operation				
(constant electrical load)				
time 200s	Total current decreased to	90%		
time 800s	Total current restored to	100%		
time 1400s	Oxidant agent decreased to	90%		
time 2000s	Oxidant agent restored to	100%		
time 2600s	Total current & oxidant agent to	90%		
time 3200s	Total current & oxidant agent to	100%		
Gas turbine in closed loop, i.e. constant speed operation				
(variable electrical load)				
time 4300s	Total current decreased to	90%		
time 4900s	Total current restored to	100%		
time 5500s	Oxidant agent decreased to	90%		
time 6100s	Oxidant agent restored to	100%		
time 6700s	Total current & oxidant agent to	90%		
time 7300s	Total current & oxidant agent to	100%		

As shown in Figure 8, the oxidant flow steps cause a change in the syngas flow to the fuel cell which is delayed because of the gasifier gas residence time, in the order of 10s.



Figure 8 – System input perturbations: fuel cell (FC) current and oxidant agent (humid air) to the gasifier.

## RESULTS

The analysis of results follow the path of the fuel: first the gasifier behavior is analyzed, then the fuel cell behavior, and finally the impact on the gas turbine cycle. However, it is anticipated that the gas turbine cycle actually feeds back its dynamic response to the fuel cell, so that the IGFC overall behavior can be understood only as a whole.

Figure 9 illustrates the syngas thermal content behavior, which is clearly affected by oxidant flow steps only. The decrease in oxidant flow makes the overall thermal output decrease (blue line), despite the lower heating value (LHV) showing an opposite behavior (magenta line). However, the useful thermal power, i.e. the syngas without tar, is much less affected: after a sudden drop, the power seems to recover, which could be a quite beneficial self-healing effect. This phenomenon is likely to be explained by the increase in combustion zone temperature (Figure 10) which follows the oxidant flow step down: the transient higher temperature causes gasification endothermic reactions to proceed further on, thus temporarily compensating the decrease of oxidant flow. As a result, the green line in Figure 9 shows a fairly stable behavior. The temperature behavior in Figure 10 well explains the overall gasifier outputs shown in Figure 9.

The gasifier is not operated in the new conditions long enough to reach a new steady-state: in fact, the large amount of biomass stored in it would require approximately between half an hour and one hour to get to a new regime. As a result, the relatively quick sequence of maneuvers build up some non-recovered mass or heat unbalance, as shown by the combustion zone temperature in Figure 10 (red line), which clearly keeps dropping on the average: this might or might not turn out to be a problem for the stability of gasifier operation, as it depends on the steps applied and the time awaited in between them. The temperature of ashes (T after combustion in Figure 10) is low because of the quenching effect due to the injected oxidant flow.



Figure 9 – Gasifier syngas thermal content (before the syngas conditioning unit).



Figure 10 – Gasifier significant temperatures.



Figure 11 – Raw syngas composition (top) and zoom in significant fuel gases (bottom).

The gas molar composition behavior (Figure 11) explains the LHV variations: when oxidant flow is reduced, the lower amount of  $N_2$  helps in elevating the LHV content of the output syngas. The decrease in  $N_2$  content is counterbalanced by an increase in the fuel gases, namely  $H_2$ , CO and CH<sub>4</sub>. The time response is dominated initially by the syngas residence time (on the order of 10s) and later by the gasifier thermal response. On the other hand,  $H_2O$  consistently shows a step change followed by a recovery trend, so that the overall amount does not significantly change along the transients. This might be explained by the fact that the steam present in the oxidant agent

is effectively used for char gasification, so that the output steam is mainly a function of the biomass humidity, which did not change in this case.

Figures 12 and 13 show the fuel cell response. Current and syngas flow steps cause the utilization factor (calculated on the output anode composition) to vary as expected: however, the variation is clearly much lower in case a 10% step in oxidant flow is applied rather than a 10% step in total current. When both steps are applied simultaneously, an initial peak is shown by the utilization factor: in fact, while the current impacts almost immediately on it, the syngas flow requires some seconds to change in flow and composition, thus providing such an apparent "peaky" behavior.



Figure 12 – Fuel cell main parameters: Nernst voltage, operating fuel cell voltage, utilization factor (Uf).

From Figure 13 it is interesting to observe a significant difference between the first 4000s and the later times. Variable speed operation, i.e. the first 4000s, cause minimal variations in the fuel cell inlet temperature, as a consequence of the almost constant recuperator outlet temperature; on the other hand, constant speed causes some thermal stress at the inlet, while mitigating the temperature oscillations at the outlet. This unexpected result can be useful for discerning which control system to adopt for the gas turbine side, depending on the most important thermal stress to be minimized within the fuel cell stack. On the other hand, the thermal spatial gradients (Figure 13, bottom) do not change significantly in amplitude between the two cases: the highest gradient remains in the centre of the cell, as a consequence of the higher current density.

Figure 14 shows the variations in mass flow and pressure: of course, variable speed involves variable air flow and variable pressure, and they are strictly linked to the gas turbine

rotational speed (Figure 15). In principle, mass flow can be decoupled from the rotational speed by operating on cold air or hot air bypass control, which did not happen this time. Thus, with reference to Figure 13, the oscillations in inlet temperature could be effectively minimized also for constant speed operation, which would have the additional advantage of relatively constant pressure operation.



Figure 13 – Fuel cell temperatures and temperature spatial gradients (along the flow axis) .



Figure 14 – Gas turbine flows and pressure.



Figure 15 – Gas turbine power and speed.

Finally, Figure 16 shows the main temperatures of the cycle. Reading the legend from top to bottom, the compressed air as delivered from the recuperators is pre-heated by the virtual heat exchanger in the fuel cell (FC) system up to fuel cell inlet temperature. The fuel cell outlet goes to the post-combustor of the anode off-gases; such a flow is meant to pre-heat the incoming air and firing the turbine, and then exit the fuel cell system. In theory, such an exit temperature (called "Simulated Comb outlet") should be the same as the actual combustor outlet (called "Actual Comb outlet, T333). They show the same behavior along the entire test, with the T333 being quite

disturbed by combustion dynamics, but with an offset of about 100K. The actual combustion outlet temperature is, however, higher than that simulated. The reasoning is that the actual heat capacity rate of the "real" reactant flows is smaller than the heat capacity rate of the "simulated" reactant flows. In order for the heat rate "Q dot" to remain consistent between simulation and actuality, higher temperatures thus manifest during experimentation.

All these aspects contribute to justify the use of additional fuel (i.e. higher temperatures) to run the system at the same conditions. However, it is important to highlight that the same dynamic behavior is retained, which is essential for the purposes of these tests.



Figure 16 – IGFC cycle temperatures.

The actual combustor outlet is actually equivalent to the TIT in case of no bypassed air. In this respect, its behavior is expected to directly impact on gas turbine dynamics: in this test, because of the large portion of bypassed cold air, the overall impact is reduced.

It can be observed that in case of parallel steps in current and oxidant flow (steps around 3000s and 7000s), T333 variations are mitigated, if compared to the steps of electrical current only (steps around 500s and 4500s), as well as the variations in turbine speed or power (Figure 15). This fact tells the opportunity in targeting the parallel control of both the gasifier and the fuel cell hybrid system together, rather than separated controllers. The development of a controller that could modulate gasifier oxidant flow in conjunction with fuel cell electrical current would be ideal for minimizing the thermal

stress to the system as well as achieving relatively quick response to load variations.

# CONCLUSIONS

The Hyper facility at NETL has been upgraded with the inclusion of a real-time gasifier model, now linked to a preliminary fuel cell model and gas turbine hardware. Such a first IGFC layout was first successfully run in July 2010. The preliminary results obtained from the analysis of some representative transients allow the following conclusions to be drawn:

- The newly developed "Generic Thermal Library" was successfully tested in the Hyper facility and run in real-time together with the fuel cell model.
- The type of gasifier analyzed here (atmospheric, updraft) shows a possible self-healing behavior which might mitigate the dynamic impact on the fuel cell performance during transient maneuvers.
- Variable speed operation minimizes the thermal stress at the fuel cell stack inlet because changes in thermal effluent from the fuel cell system result in a corresponding change in turbine speed and compressor inlet flow. This insures that thermal energy and mass flow track each other to maintain a more stable temperature at the fuel cell inlet. Cathode mass flow could then be maintained through modulation of either the hot or cold air bypass valves. The disadvantage to this approach would be the variations in cathode pressure as a result of the transient turbine speed.
- Since a fuel cell thermal output change does not result in a change in compressor mass flow under synchronous turbine speed operation, cathode inlet temperature control would require supplementary heating. The advantage to synchronous operation is that cathode pressure and mass flow can be maintained through load and gasifier output transients.
- The advantage of having a parallel controller of both the gasifier and the fuel cell gas turbine hybrid system based upon load demand (i.e. fuel cell current) has been identified.

Future developments in this work regard the population of an experimental database with more tests, in order to improve the insight into the IGFC dynamics. After more confidence is achieved in system operation and control, a more efficient setting in the operating parameters (i.e. also more sensitive to external disturbances) can be implemented, including a different gasifier concept, such as an oxygen blown entrained flow gasifier, which is more typical for large energy plants.

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