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Kelly, Nick and Ferguson, Alex and Griffith, Brent and Weber, Andreas (2008) *The development of a generic systems-level model for combustion-based domestic cogeneration.* In: Micro-Cogen 2008, 1st International Conference on Micro-Cogeneration Technologies and Applications, 2008-04-29 - 2008-05-01, Ottawa, Canada.

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THE DEVELOPMENT OF A GENERIC SYSTEMS-LEVEL MODEL FOR COMBUSTION-BASED DOMESTIC COGENERATION

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ABSTRACT

The provision of heat and power to dwellings from micro-cogeneration systems is gaining credence around the developed world as a possible means to reduce the significant carbon emissions associated with the domestic sector. However, achieving the optimum performance for these systems requires that building design practitioners are equipped with robust, integrated models, which will provide a realistic picture of the cogeneration performance in-situ.

A long established and appropriate means to evaluate the energy performance of buildings and their energy systems is through the use of dynamic building simulation tools. However, until now, only a very limited number of micro-cogeneration device models have been available to the modelling community and generally these have not been appropriate for use within building simulation codes. This paper describes work undertaken within the International Energy Agency's Energy Conservation in Building and Community Systems Annex 42 to address this problem through the development of a generic, combustion-based cogeneration device model that is suitable for integration within building simulation tools and can be used to simulate the variety of Internal Combustion Engine (ICE) and Stirling Engine (SE) cogeneration devices that are and will be available for integration into dwellings.

The model is described in detail along with details of how it has been integrated into the ESP-r, EnergyPlus and TRNSYS simulation platforms.

OVERVIEW

Annex 42 of the International Energy Agency's Energy Conservation in Buildings and Community Systems Programme (IEA/ECBCS) was established to investigate the performance residential cogeneration systems. One of the principal aims of the Annex was to develop the models needed to support the building simulation and wider building design community in the technical analysis of this emerging technology. This paper describes the development of one of these models developed for the simulation of Internal Combustion Engine (ICE) or Stirling Engine (SE) micro-cogeneration devices.

A review undertaken by the Annex indicated that prior to its formation there had been few attempts to model residential cogeneration in detailed building simulation tools. McRorie et al (1996) and Kelly (1998) developed models of medium-scale ICE-based cogeneration devices; however neither model was appropriate for the modelling of domestic cogeneration. Pearce et al. (1996, 2001) studied the annual performance of Stirling engines but their modelling approach neglected the effects of different control strategies and thermal storage, which are of interest when investigating the integration of this technology in residential buildings.

Despite the lack of building-simulation specific models, the literature was rich with SE and ICE models developed for general analysis of cogeneration devices. However, the majority of the models reviewed had been developed for the analysis of engine phenomena occurring over very short time scales (10^{-3} to 10^{-6} seconds) making their integration into building simulation codes (operating using time scales many orders of magnitude longer - 10 to 10^3 seconds) an impractical proposition.

In view of the lack of available models, the Annex's models were developed from first principles, rather than being developed from existing code. A pragmatic "grey box" modelling approach was adopted; where the model structure reflected the underlying physical system and where individual constituents (e.g. heat exchanger) were described using one or more control volumes: A control volume being an arbitrary bounded

region of space to which the laws of conservation of mass, momentum, species and energy can be applied. Conservation equations can be derived for each volume, forming the basis for solution of the time-varying energy and mass flows within a device. The form and input parameters for the individual model equations were derived from comparison with easily obtainable empirical data or extracted from more detailed models. This approach is used extensively in many areas of engineering modelling (e.g. Clarke, 2001; Hrovat and Sun, 1997). This modelling approach led to the form of model described in this paper, which can be modified to represent any combustion-based cogeneration device.

MODEL ENERGY EQUATIONS

The cogeneration model comprises three basic control volumes (figure 1):

1. the *energy conversion control volume* represents the engine working fluid, combustion gases and engine alternator, this control volume feeds information from an engine unit performance map (in the form of a heat flux) into a thermal model;

2. the *engine control volume* represents the aggregated thermal capacitance associated with the engine block and the majority of the heat exchangers' thermal capacitance; and

3. the *cooling water control volume* represents the cooling water flowing through the device and the elements of the heat exchanger in immediate thermal contact.

This form of model emerged from an iterative development/calibration process described elsewhere (Beausoleil Morrison and Kelly [eds.], 2007). The energy conversion control volume enables the part-load performance of the device to be calculated, while the thermal mass and cooling water control volumes facilitate the modelling of the transient thermal performance.

Energy Conversion Control Volume

This represents the combustion processes taking place within (or outside in the case of Stirling engines) the cylinder or cylinders of the engine unit. The steady-state energy balance for this volume is:

$$\dot{H}_{fuel} + \dot{H}_{air} = P_{net,ss} + q_{gen,ss} + \dot{H}_{exh} \qquad (1)$$

The model does not attempt to fully characterize the energy balance described by equation 1. Instead, the engine's steady-state (part load) performance is correlated to the total energy input to the system:

$$P_{net,ss} = \eta_e q_{gross} \qquad (2)$$

$$q_{gen,ss} = \eta_q q_{gross} \qquad (3)$$

$$q_{gross} = \dot{m}_{fuel} \cdot LHV_{fuel} \qquad (4)$$
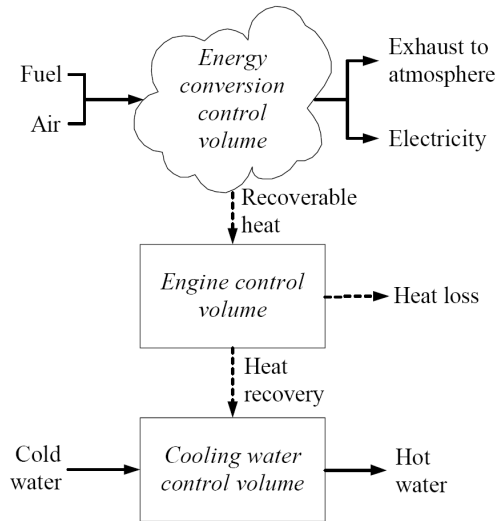
Figure 1: the generic engine model control volumes.

These performance equations rely upon the electrical and thermal efficiencies and relate useful energy production to fuel energy consumption. The efficiencies are assumed to be functions of the electrical output, coolant flow rate and temperature: this approach has significant advantages over a more detailed model - its simplicity, ease of calibration and reduced data collection burden. However the model must be calibrated using empirical data and so specific instances of the model are applicable to only one engine type, capacity, and fuel type.

$$\eta_e = f(\dot{m}_{cw}, T_{cw,i}, P_{net,ss}) \qquad (5)$$

$$\eta_q = f(\dot{m}_{cw}, T_{cw,i}, P_{net,ss}) \qquad (6)$$

The two efficiency correlations constitute a "performance map" describing the CHP system's steady-state behaviour under a variety of loading conditions.

The lower-heating value term of the fuel given in equation 4 is determined by summing the enthalpies of formation of all reactants and products associated with the device's combustion process[1] and assuming that all of the water in the combustion products is in vapour form:

$$LHV_{fuel} = \frac{\sum\limits_{reactants} \chi_i \hat{h}_i^o - \sum\limits_{products} \chi_i \hat{h}_i^o}{\sum\limits_{reactants} M_i} \qquad (7)$$

The model supports the fuel constituents given below.

Table 1: supported fuel constituents

Fuels	
hydrogen (H2)	
hydrocarbons	methane (*CH*4) ethane (*C2H6*) propane (*C3H*8) butane (*C4H*10) pentane (*C5H*12) and hexane (*C6H*14)
alcohols	methanol (*CH3OH*) and ethanol (*C2H5OH*)
inert constituents	carbon dioxide (*CO2*) and nitrogen (*N2*) and oxygen (*O2*)

Engine and Cooling Water Control Volumes and the Modelling of Thermal Transients

The dynamic thermal behaviour of the model is characterized by the thermal mass of its engine block and encapsulated working fluid, internal heat exchange equipment, and in the case of SE-based technology, the external heater. Since the model lacks the resolution

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[1] The enthalpies of formation ($\hat{h}_i^o$) should be evaluated at 25°C for all constituents.

---

required to characterize the thermal response of these individual subcomponents, they are represented using a single, homogeneous thermal mass control volume. The thermal energy stored within this control volume is quantified using an aggregate thermal capacitance, $[MC]_{eng}$, (J/K) and an equivalent average engine temperature T_{eng} (°C)

The energy balance of the engine control volume is:

$$[MC]_{eng} \frac{dT_{eng}}{dt} = UA_{HX}\left(T_{cw,o} - T_{eng}\right) \qquad (8)$$
$$+ UA_{loss}\left(T_{room} - T_{eng}\right) + q_{gen,ss}$$

The heat exchanger control volume energy balance also includes heat storage and so the energy balance of the cooling water control volume is also represented by a 1st order differential equation:

$$[MC]_{cw} \frac{dT_{cw,o}}{dt} = [\dot{m}c_p]_{cw}\left(T_{cw,i} - T_{cw,o}\right) \qquad (9)$$
$$+ UA_{HX}\left(T_{eng} - T_{cw,o}\right)$$

The parameters required to calibrate the model's governing equations (1)-(9) can be determined from non-intrusive bench testing of a cogeneration device (e.g. measurement of fuel flow rate, cooling water flow rates and temperature, electrical production).

CONTROL OF THERMAL / ELECTRICAL OUTPUT

The electrical output of the model can be controlled explicitly, where the power required is specified by the host simulation code. The required electrical output defines the operating point of the device ($P_{net,ss}=P_{demand}$) and is the starting point for the solution of equations (1)-(9). Note that modulation of the electrical output also enables the thermal output of the device to be varied hence a separate thermal control mechanism was not required.

MODELLING THE CONSTRAINTS TO DEVICE BEHAVIOUR

Equations (1)-(9) describe the behaviour of the device while operating under normal conditions, producing heat and power. However, these core energy balance equations need to be supplemented by additional performance information as very often the device behaviour is dictated not by thermodynamics but by the action of on-board (or internal) controls. These controls ensure that the optimum performance is achieved for a given set of operating conditions, and that the unit's

safe range of operation is not exceeded; they are explicitly represented in the model as follows.

Operational Cycling

One of the most important aspects of residential cogeneration behaviour is cycling between different modes of operation. Cogeneration devices may exhibit three other operating modes other than normal operation with markedly different characteristics: standby, warm-up and cool-down.

<u>Standby</u> - in this mode the unit consumes no fuel and produces no heat. However, the electronic controllers within the unit require some power while awaiting activation (supplied from the grid). Thus:

$$
\begin{aligned}
P_{net,ss} &= P_{net,standby} \\
q_{gen,ss} &= 0 \\
\dot{m}_{fuel} &= 0
\end{aligned}
\tag{10}
$$

<u>Warm-up</u> - Stirling engines may exhibit a pronounced warm-up period, in which the fuel flow and electric output differ considerably from their steady-state values. To account for this some model characteristics are correlated to a *nominal engine temperature* - which is assumed to represent conditions in the engine under steady-state conditions. The engine's fuel flow during warm-up is:

$$
\dot{m}_{fuel,warm-up} = \dot{m}_{fuel,ss-max} \\
+ k_f \dot{m}_{fuel,ss-max} \left(\frac{T_{eng,nom} - T_{room}}{T_{eng} - T_{room}} \right)
\tag{11}
$$

Similarly the power produced during warm-up is given by:

$$
P_{net,warm-up} = P_{max} k_p \left(\frac{T_{eng} - T_{room}}{T_{eng,nom} - T_{room}} \right)
\tag{12}
$$

The warm-up characteristics of internal combustion engines are not sensitive to engine temperature. However, these devices may exhibit a static time delay between activation of the unit and power generation. The power generated by these devices is determined as:

$$
P_{net,warm-up} \\
= \begin{cases} 0 & \text{if } (t - t_o) < t_{warm-up} \\ P_{demand} & \text{if } (t - t_o) \geq t_{warm-up} \end{cases}
\tag{13}
$$

<u>Cool-down</u> - in this mode the engine is assumed to consume no fuel and generate no heat, however as in the case of the warm-up mode the auxiliary electrical systems in the engine may require additional power to complete the shutdown. Thus:

$$
\begin{aligned}
P_{net,ss} &= P_{net,cool-down} \\
q_{gen,ss} &= 0 \\
\dot{m}_{fuel} &= 0
\end{aligned}
\tag{14}
$$

The model tracks which operating mode the CHP unit is currently in and switches the unit between modes depending on the prevailing system state.

Coolant Flow Control

Some cogeneration devices are equipped with an internal valve, allowing them to regulate the flow rate of the cooling water and optimize engine performance and heat recovery (Zilch, 2005). An additional empirical correlation is provided within the model to account for this:

$$
\begin{aligned}
\dot{m}_{cw} &= c_0 + c_1 P_{net,ss}^2 + c_2 P_{net,ss} \\
&+ c_3 T_{cw,i}^2 + c_4 T_{cw,i} \\
&+ c_5 P_{net,ss}^2 T_{cw,i}^2 + c_6 P_{net,ss} T_{cw,i} + c_7 \\
&+ c_8 P_{net,ss}^2 T_{cw,i}
\end{aligned}
\tag{15}
$$

The air stoichiometry can be similarly regulated to manage the CHP unit's combustion efficiency, operating temperature and emissions:

$$
\begin{aligned}
\dot{m}_{air} &= f(\dot{m}_{fuel}) \\
&= d_0 + d_1 \dot{m}_{fuel}^2 + d_2 \dot{m}_{fuel}
\end{aligned}
\tag{16}
$$

Rate Limiting

Internal controllers may restrict the rates at which the fuel flowing to the system can be increased and decreased. In the absence of detailed models describing these controllers, the model allows constraints on the

maximum rate of change permitted in the system fuel flow using empirically derived data are as follows:

$$\dot{m}_{fuel}^{t+\Delta t}$$
$$= \begin{cases} \dot{m}_{fuel,demand}^{t+\Delta t} & d\dot{m}_{fuel}/dt \le \left(d\dot{m}_{fuel}/dt\right)_{max} \\ \dot{m}_{fuel}^{t} \pm \left(d\dot{m}_{fuel}/dt\right)_{max} & d\dot{m}_{fuel}/dt > \left(d\dot{m}_{fuel}/dt\right)_{max} \end{cases}$$

(17)

The model also includes the option to constrain the device's electrical output. The rate of change in the cogeneration unit's power output is compared to a specified maximum rate of change derived from empirical data, and adjusted to reflect the unit's transient characteristics:

$$P_{net}^{t+\Delta t}$$
$$= \begin{cases} P_{net,ss}^{t+\Delta t} & dP_{net}/dt \le \left(dP_{net}/dt\right)_{max} \\ P_{net}^{t} \pm \left(dP_{net}/dt\right)_{max} & dP_{net}/dt > \left(dP_{net}/dt\right)_{max} \end{cases}$$

(18)

Maximum and Minimum Output

The cogeneration unit's range of operation can be bounded by two operating points corresponding to the system's maximum and minimum output. If the controller requests an output exceeding the system's maximum output operating point, the system should be operated to produce its maximum output. If the controller requests an output less than the system's minimum output operating point, the system will be either i) operated to produce its minimum output, or ii) deactivated.

Overheating Protection

The model also allows for deactivation of the device when dangerous operating conditions are detected such as low cooling water flow rate or high cooling water temperature.

CO$_2$ EMISSIONS

The model provides a functional CO$_2$ emission equation that assumes complete combustion of the hydrocarbon fuel:

$$\dot{m}_{CO_2} = \left(\frac{\dot{m}_{fuel}}{\sum_{fuel\,constituents} \chi_i MM_i} \right) \left(\sum_{fuel\,constituents} \chi_i n_{C,i} \right) MM_{CO_2}$$

(19)

VALIDATION AND CALIBRATION

Within Annex 42 the model described has been successfully calibrated using data from both ICE and SE performance data; it has also been extensively validated using empirical data and through a rigorous programme of inter-model comparison. These activities are described in detail by Beausoleil-Morrison and Ferguson [eds.] (2007).

As an example of the performance of the model, figure 2 shows the predictions of a version of the model calibrated to represent a 5.5kW ICE device against independent experimental data.

IMPLEMENTATION

The combustion device model has been integrated into three commonly used building simulation platforms. These are as follows.

- *ESP-r* - The device model has been integrated into the current release of the ESP-r platform, taking the form of an algorithm (a coefficient generator which integrates the device within the ESP-r matrix-based systems solver) and corresponding database entry, which holds the data for the specific implementation of the device. ESP-r is available for download at www.esru.strath.ac.uk

- *TRNSYS* - The model has been developed as user defined TRNSYS Type, based on the ESP-r coefficient generator subroutines. However the model was adapted to the component-based solution approach prevalent within TRNSYS. The Type is available upon request from EMPA Building Technologies (www.empa.ch).

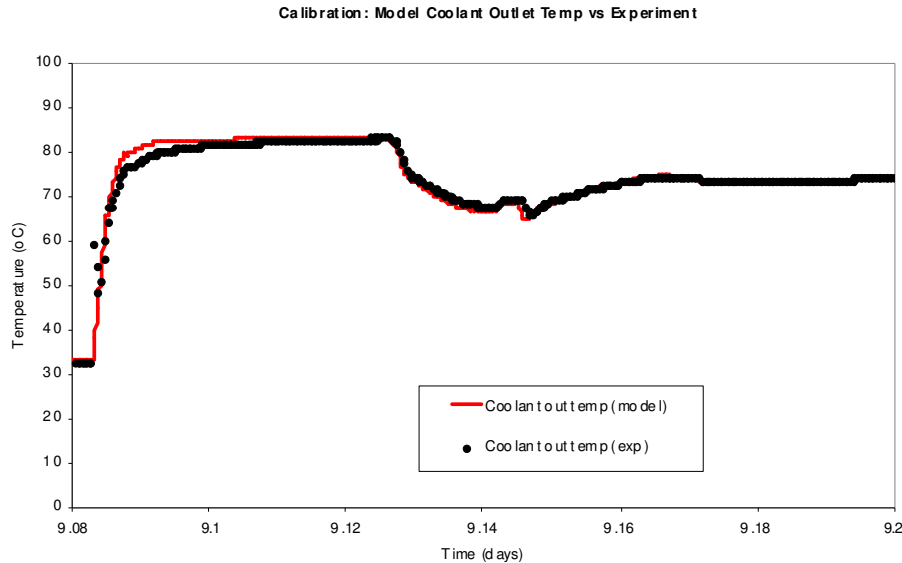**Calibration: Model Coolant Outlet Temp vs Experiment**

Figure 2: 5.5kW ICE model predictions against measurements from an independent experimental dataset.

- *EnergyPlus* - The combustion model (both ICE and SE) are accessed using the input object called GENERATOR:MICRO CHP. For more information refer to the EnergyPlus documentation; EnergyPlus is available for download at the Web site www.energyplus.gov.

CONCLUSION

A generic residential cogeneration model has been developed within IEA ECBCS Annex 42 that can be applied to a wide variety of combustion-based cogeneration devices and has been designed with considerable flexibility in mind (a feature inherent in the underlying modelling approach).

Calibrated, validated versions of the model have been successfully integrated into a three commonly used building simulation codes and used in some of the Annex's investigations into residential cogeneration performance (e.g. Dorer et al. [2007]).

With regards to further development of the model, pollutant emissions such as SO_x and NO_x are not dealt with in detail. The combustion engine models incorporate a form of equation suitable for the modelling of time-varying non-CO_2 pollutant emissions. However, no attempt has been made to calibrate and validate these equations.

The model does not explicitly consider the heat transfer to the cooling water in a device's exhaust gas heat exchanger. Instead, it aggregates these effects into an overall heat transfer modulus (UA_{HX}). This approach clearly reduces the complexity of the model and introduces some error, but the experiments conducted within Annex 42 did not include the invasive instrumentation necessary to separately characterize the engine-jacket and exhaust-gas heat transfer.

Finally, these models are intended for use at time steps ranging from 1 second up to a few minutes. Half-hourly or hourly time-steps are not recommended were transient issues are a concern as their accuracy could be compromised.

ACKNOWLEDGEMENTS

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NOMENCLATURE

$\dot{H}_{fuel}$	inlet enthalpy rate of the fuel (W)
$\dot{H}_{air}$	inlet enthalpy rate of the combustion air (W)
$\dot{H}_{exh}$	exit enthalpy rate of the exhaust gases (W)
$\hat{h}_i^o$	enthalpy of formation of constituent i at STP (J/kg or J/kmol)
k_p	empirical coefficient (-)
k_f	empirical coefficient (-)
LHV_{fuel}	lower heating value of the fuel (J/kg or J/kmol)
M_i	molar mass of constituent i. (kg/kmol)
$\dot{m}_{cw}$	mass flow rate of the cooling water (kg/s)
$[MC]_{cw}$	thermal capacitance of the cooling water control volume (J/K)
$[MC]_{eng}$	thermal capacitance of the control volume (W/K)
$\dot{m}_{fuel}$	rate of fuel flow calculated by the model at some time t (kg/s)
$\dot{m}_{fuel,warm-up}$	rate of fuel flow during warm up (kg/s)
$\dot{m}_{fuel,ss-max}$	maximum rate of fuel flow to the device under steady state (kg/s)
$\dot{m}_{air}$	combustion air flow rate (kg/s)
$[\dot{m}c_p]_{cw}$	thermal capacity flow rate of the cooling water (W/K).
$\dot{m}_{CO_2}$	the mass flow rate of CO_2 emitted by the unit (kg/s)
MM_i	the molar mass of fuel constituent i (kg/mol)
MM_{CO_2}	the molar mass of CO_2 (kg/mol)
$n_{C,i}$	the number of mols of carbon in a single mol of constituent i
P_{demand}	electricity demand of the dwelling (W)
P_{max}	maximum power output of the device (W)
P_{net}	rate electricity absorbed or produced by the device (W)
$P_{net,ss}$	rate of steady state electricity production (W)
$P_{net,cool-down}$	power used by the unit's control systems while in standby operation

	(W)
$P_{net,standby}$	power used by the unit's control systems in standby operation (W)
$P_{net,warm\ up}$	rate of power generation during warm up conditions (W)
$\left(dP_{net}/dt\right)_{max}$	maximum rate of change in the electrical output (W/s)
q_{gross}	gross heat input (W)
$q_{gen,ss}$	Steady state rate of heat generation within the engine (W)
q_{HX}	rate of heat transfer to the cooling water (W)
$q_{skin-loss}$	rate of heat loss from the unit (W)
t	time (s)
Δt	duration of the simulation time step (s)
$t_{cool-down}$	duration of the cool-down period (s)
t_o	time at which the engine was started (s)
$t_{warm\ up}$	static delay between activation and power generation (s)
$T_{cw,i}$	temperature at the inlet of the cooling water control volume (^{o}C)
$T_{cw,o}$	bulk exit temperature of the encapsulated cooling water and shell (^{o}C),
T_{eng}	bulk temperature of the thermal mass control volume (^{o}C)
$T_{eng,nom}$	nominal engine temperature (^{o}C)
T_{room}	temperature of surrounding space (^{o}C)
$\dot{m}_{fuel}$	fuel flow rate (kg/s or kmol/s)
$\dot{m}_{fuel,demand}^{t+\Delta t}$	system fuel flow rate requested by a high level control (kg/s)
$\left(d\dot{m}_{fuel}/dt\right)_{max}$	maximum rate of change in the system fuel flow rate (kg/s^2)
UA_{HX}	thermal conductance between engine and cooling water control (W/K) volumes,
UA_{loss}	thermal conductance between the engine and surroundings (W/K)

η_e	steady state electrical conversion efficiency of the engine (-)
η_q	steady state part load, thermal efficiency of the engine (-)
χ_i	molar fraction of constituent i, (-)