Improving Ethanol Life Cycle Energy Efficiency by Direct Utilization of Wet Ethanol in HCCI Engines

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Homogeneous charge compression ignition (HCCI) is a new engine technology with fundamental differences over conventional engines. HCCI engines are intrinsically fuel flexible and can run on low-grade fuels as long as the fuel can be heated to the point of ignition. In particular, HCCI engines can run on "wet ethanol:" ethanol-in-water mixtures with high concentration of water. Considering that much of the energy required for processing fermented ethanol is spent in distillation and dehydration, direct use of wet ethanol in HCCI engines considerably shifts the energy balance in favor of ethanol. The results of the paper show that a HCCI engine with efficient heat recovery can operate on a mixture of 35% ethanol and 65% water by volume while achieving a high brake thermal efficiency (38.7%) and very low NO_x (1.6 ppm, clean enough to meet any existing or oncoming emissions standards). Direct utilization of ethanol at a 35% volume fraction reduces water separation cost to only 3% of the energy of ethanol and coproducts (versus 37% for producing pure ethanol) and improves the net energy gain from 21% to 55% of the energy of ethanol and coproducts. Wet ethanol utilization is a promising concept that merits more detailed analysis and experimental evaluation.
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Introduction

Ethanol has been promoted as a domestically produced biofuel that could reduce both CO_2 emissions and dependence on foreign oil. However, a lively debate exists on the actual benefits of ethanol production and consumption. Ethanol critics have reported that up to 70% more energy is required to produce ethanol than the energy it contains [1]. Environmental consequences of ethanol production, such as soil degradation, have also been described and quantified. The high cost of ethanol production has also been criticized, and it is typically recognized that ethanol production in the USA is dependent on government subsidies to be competitive. Ethanol utilization is also promoted through legislation that mandates the use of oxygenated and alternative fuels.

The energy balance of ethanol has been studied in detail. Recent publications [2,3] have reported a slight energetic advantage from producing and using ethanol from corn. Figure 1 illustrates the results of the energy balance for corn ethanol including coproducts (corn gluten and oil). In this figure, the circle represents the total energy of ethanol and coproducts. Out of this energy, substantial fractions are spent in ethanol distribution (2%), corn production (fertilizers and fuel for farming equipment, 22%), corn transportation (3%), mashing and cooking (16%), distillation (23%), and dehydration (14%). The net energy gain is 21%, which includes 15% of energy in coproducts and 6% energy surplus in ethanol. The net energy gain is likely to increase in the future due to improved farming and processing techniques [3].

Another possibility for improving the energy balance of ethanol is developing new utilization techniques that may reduce the energetic cost of converting ethanol to a useful form. Figure 1 shows that the greatest fraction of the energy necessary for making ethanol is spent in water removal (distillation and dehydration; 37% of the total energy in ethanol and coproducts). Reducing the energy spent in water removal may therefore considerably improve the ethanol energy balance.

Figure 2 shows the energetic cost of ethanol distillation as a function of the final ethanol concentration, assuming that the process starts with a 12% ethanol-in-water mixture produced by fermentation [4]. Previous research [5] determined the energy necessary to distill an ethanol-water mixture from 80% to 96% volume fraction. Below 80%, we assume that distillation energy scales linearly with ethanol concentration down to the initial 12%. Figure 2 shows that the energy required for distillation increases slowly at first, reaching 10% of the lower heating value at about 80% concentration. As the concentration approaches the azeotrope (95.6%), the distillation energy increases rapidly to extremely high values. At this point, it is desirable to stop the distillation process and separate the remaining water through dehydration.

It is apparent from Fig. 2 that considerable energy savings can be achieved through utilization of wet ethanol with partial water removal. For example, if ethanol can be used at a 35% volume concentration, the energy required for distillation would drop from 23% to 3% of the energy of ethanol and coproducts. Use of wet ethanol would also avoid the need for dehydration. While many applications may demand pure ethanol (for example, ethanol as a gasoline additive), finding a practical application for wet ethanol may make the overall energy balance much more attractive.

Prime movers typically available for transportation and for distributed power generation (spark-ignited (SI) and diesel engines) do not perform well with wet ethanol. Combustion in SI engines occurs through propagation of a flame that initiates at the spark plug and spreads through the combustion chamber. High concentrations of water in the fuel result in substantial dilution of the fuel-air mixture. Excessive dilution slows down the propagation of the flame, resulting in misfire. In addition to this, SI engines need to operate at low compression ratio (less than ~11) and low intake temperature (less than ~60°C) to avoid knock. The low compression ratio limits the engine efficiency and the low intake

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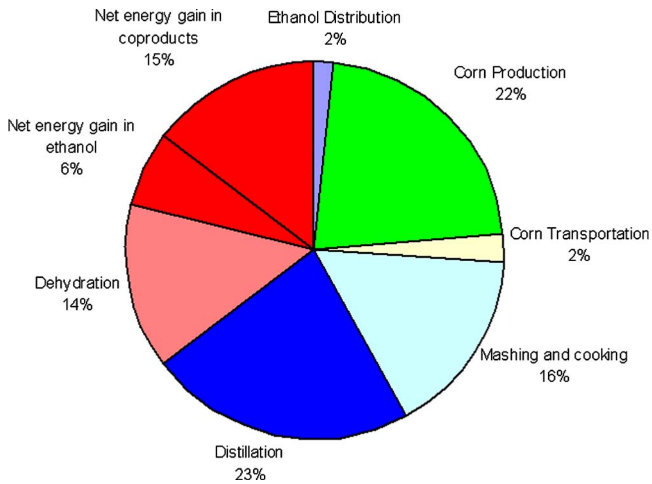

Fig. 1 Net energy balance for ethanol [2,3]. The full circle represents the energy output of ethanol and coproducts. The figure shows wedges indicating energy consumption in all stages of ethanol production from corn, as a percent of the heating value of ethanol and coproducts. The energy that remains after accounting for all the energy consumption is the net energy gain, which has two components: net energy in the ethanol and net energy in the coproducts.

temperature limits the humidity of the intake gases, because condensation in the intake may damage engine components or mix with oil and reduce its lubricity.

It is also difficult to run a diesel engine on wet ethanol. Pure ethanol itself is not a good fuel for diesel engines due to its high resistance to autoignition (high octane number and low cetane number). Resistance to autoignition increases if wet ethanol is used, because water inhibits chemical reaction by cooling down the air inside the combustion chamber as it evaporates. Therefore, it is difficult to obtain appropriate combustion of wet ethanol in a diesel engine in the short time available for combustion.

It may be possible to run SI or diesel engines on wet ethanol if the water concentration is low (a few percent). Establishing the maximum water concentration that allows efficient SI and diesel engine operation is an important task that merits further research because direct use of even slightly wet ethanol could save considerable distillation and dehydration energy (Fig. 2).

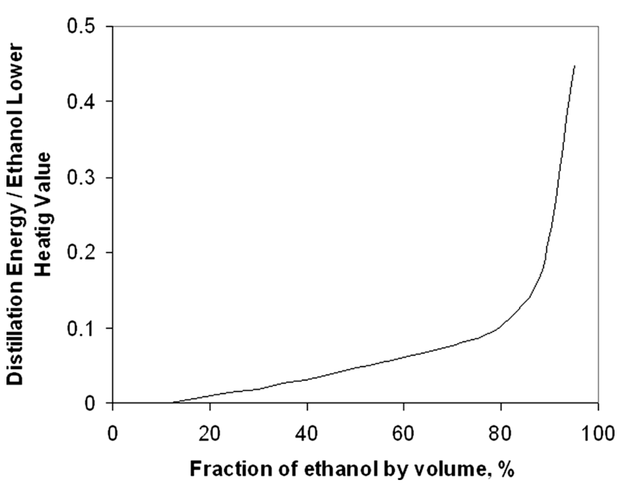

Fig. 2 Energy required for ethanol distillation, as a fraction of the lower heating value of ethanol, as a function of the ethanol-in-water concentration by volume after distillation. It is assumed that the concentration of ethanol at the beginning of the distillation process is 12% by volume.

For wet ethanol, another engine combustion technology may be well suited. Homogeneous charge compression ignition (HCCI) engines are a new option for prime mover in transportation and stationary applications. HCCI combustion is fundamentally different from combustion in SI engines and diesel engines. HCCI combustion is a thermal autoignition of a premixed fuel-air mixture, with no flame propagation (as occurs in SI engines) or mixing-controlled combustion (as in diesel engines) [6]. HCCI engines are intrinsically fuel flexible. Any fuel can be used as long as it can be evaporated and then heated by compression to a temperature hot enough for autoignition (approximately 1100 K [7]). The operating limits for HCCI are therefore set by the requirement to heat up the fuel and not by the need to propagate a flame across the combustion chamber. Also, fuel can be evaporated outside the engine in a vaporizer heated by exhaust gases with no direct injection of liquid fuel into the engine, so that the cooling effect of water vaporization does not have a negative effect on ignition, as it does in a diesel engine.

HCCI engines can therefore burn water-ethanol mixtures that cannot be burned in either diesel or SI engines. Unlike SI engines, HCCI engines are not limited to low intake temperature or low compression ratio due to knock. In fact, HCCI engines require a high intake temperature for ignition to occur, and HCCI engines may be described as a continuously knocking engine where the harmful effects of knock have been avoided by keeping a low combustion temperature [8]. HCCI engines can operate at high intake temperature, avoiding water condensation. They are likely to be more efficient than SI engines due to their higher compression ratio, and do not require spark plugs or a three-way catalyst and may therefore have lower maintenance costs than SI engines. Finally, HCCI engines can run extremely lean (equivalence ratio ~ 0.2) or very dilute (residual gas fraction ~ 0.6). In either case, the combustion temperature is low enough that the engine produces extremely low NO_x emissions (well below the most strict emissions standards for stationary and transportation applications) with no need for aftertreatment.

Despite the potential advantages, HCCI engines do present some technical challenges that have so far kept them from widespread commercialization. The main hurdles are combustion timing control, low specific power, high emissions of hydrocarbon (HC) and carbon monoxide (CO), and difficulty to start when cold [6]. Out of these, combustion control appears to be the greatest technical challenge, especially for transportation applications, due to the fast transients required to meet the road load. Much research is being devoted to this topic (for example, see Refs. [9–11]), and the availability of fast computer controls is making this problem tractable. Low power output is being handled with high intake pressures (3 bars or higher). Emissions of HC and CO can be controlled with commercially available technology (oxidizing catalyst). Finally, the HCCI engine can be started by running it in spark-ignited or diesel mode, and then transitioning to HCCI mode once the engine is hot [12]. However, this may require a small amount of a secondary fuel (e.g., pure ethanol), because the engine will not operate well in SI or diesel modes with wet ethanol. For stationary applications, the startability problem is easier, as external components (i.e., a burner and heat exchanger [13]) can easily be installed; these startup strategies may not be practical in transportation application because of packaging restrictions.

We propose the hypothesis that a HCCI engine can run efficiently on wet ethanol fuel and that utilizing wet ethanol fuel in HCCI engines improves the energy balance of ethanol production. We evaluate the validity of this hypothesis with an engine system model that includes a chemical kinetic HCCI engine combustion model. These models are next described followed by the analysis results, where we determine the minimum ethanol concentration (that is, the minimum level of distillation) that would allow efficient HCCI engine operation. Operating at this condition mini-

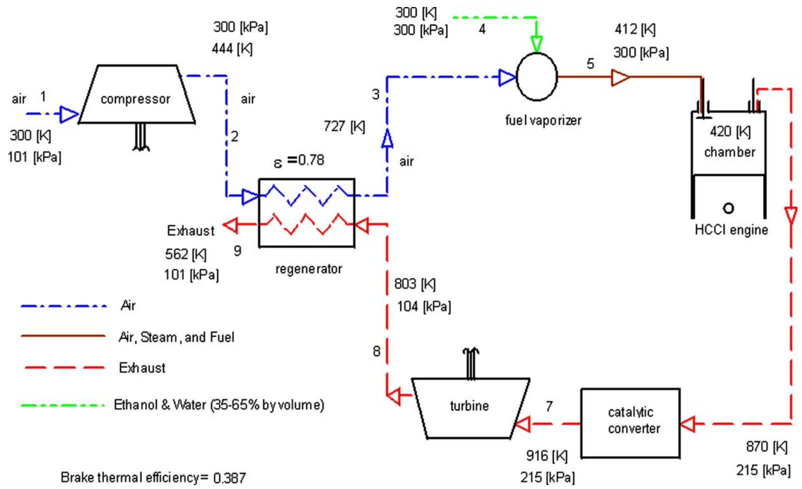

Fig. 3 Schematic of the HCCI engine system operating on wet ethanol. The numbers in the figure show pressures and temperatures for operation with a 35% ethanol in water by volume mixture as the supplied fuel. The 420 K temperature inside the engine refers to the charge temperature at the beginning of the compression stroke.

mizes the energy required for ethanol processing, improving the energy balance for ethanol and maximizing the overall system efficiency.

Note that we focus on corn as the most common source of ethanol in the USA. However, all ethanol produced by fermentation of agricultural products results in ethanol-in-water mixtures with high water content. Any potential distillation or dehydration savings found with wet ethanol are applicable to ethanol production from other agricultural feedstocks.

Engine System Model and Homogeneous Change Compression Ignition Combustion Model

Figure 3 shows a schematic of the HCCI engine system. The system is similar to what would typically be used in heavy trucks or stationary engine applications, except that we have added a regenerator for heat transfer from the exhaust into the intake gases, and a vaporizer to evaporate the fuel (and all the water mixed with it) prior to entering the combustion chamber. The system is analyzed under the following set of assumptions.

1. The HCCI combustion process is represented by a time-dependent, variable-volume, well-mixed reactor.
2. Detailed chemical kinetics predict ignition in the HCCI engine.
3. Combustion efficiency is determined by an empirical correlation.
4. Fuel and water are fully vaporized prior to entering the engine combustion chamber.
5. The volumetric efficiency of the engine is 100%, meaning the volume of air and fuel inducted into the engine cylinder is equal to the displacement of that cylinder ([14], Chap. 2).
6. Thermal losses in ducts are negligible.
7. Pressure drop in heat exchangers and ducts is negligible.
8. Turbocharger mechanical losses are neglected.

In addition, the engine is assumed to operate at a constant engine speed (1800 rpm) and nonvarying load. The problem of transitioning between different speed or load operating points is not considered. The constant speed and load assumptions mainly apply to engines in stationary power generation applications. Additional physical models would be needed to analyze the dynamics of transient operation for transportation applications. However, performance of the wet ethanol HCCI engine operating at maximum power output, applicable to stationary power or transportation engines, can be predicted without considering speed or load transients. Thus, our assumptions allow for investigation of the viability and performance of the wet ethanol HCCI engine concept.

Engine characteristics are listed in Table 1. The dimensions of the engine correspond to the Caterpillar 3406 engine, which is the subject of an ongoing HCCI stationary power generation experiment [15]. We next describe the models used for analyzing the different system components.

Turbocharger. Inducted air first flows through a turbocharger compressor. We assume that the turbocharger pressure ratio is 3. This pressure ratio is comparable to those used at maximum power in current diesel engines, and is necessary to compensate for the low specific power typical of HCCI operation. The compressor has the additional effect of heating the engine charge. Equation (1) relates conditions upstream (State 1 in Fig. 3) and downstream (State 2) of the compressor,

$$T_2 = T_1\left(\frac{P_2}{P_1}\right)^{\gamma_1 - 1/\gamma_1 \eta_{pc}} \tag{1}$$

where γ_1 is the specific heat ratio c_p/c_v in State 1, and η_{pc} is the polytropic efficiency, assumed equal to 0.8 [16]. A polytropic efficiency of 80% corresponds to an isentropic efficiency in the range of 55–70%, which is typical of automotive compressors [14]. For the turbine, we use an expression similar to Eq. (1), with the same polytropic efficiency $\eta_{pt}=0.8$.

Table 1 Main characteristics of the Caterpillar 3406 6-cylinder engine used for the HCCI analysis

Displaced volume per cylinder	2400 cm^3
Bore	137 mm
Stroke	165 mm
Connecting rod length	262 mm
Geometric compression ratio	16:1
Engine speed	1800 rpm
Engine volumetric efficiency	100%
Engine intake pressure	3 bars

$$T_8 = T_7\left(\frac{P_8}{P_7}\right)^{(\gamma_6-1)\eta_{pt}/\gamma_6} \tag{2}$$

Compressor and turbine work are calculated from enthalpy balances: $W_c=H_2-H_1$ and $W_t=H_7-H_8$. We assume no mechanical losses in the turbocharger, and $W_c=W_t$.

Regenerator. Air flowing out of the compressor is directed to a regenerator (an exhaust to intake air heat exchanger) that preheats the intake air with the exhaust gases. Intake preheating is necessary for complete ethanol-in-water mixture evaporation in the vaporizer (described in the following section). The performance of the regenerator is specified through its effectiveness defined as

$$\varepsilon_h = \frac{(\dot{m}c_p)_2(T_3-T_2)}{(\dot{m}c_p)_{\min}(T_8-T_2)} \tag{3}$$

where subscripts 2, 3, and 8 indicate locations in Fig. 3, and $(mc_p)_{\min}$ is the minimum of $(mc_p)_2$ and $(mc_p)_8$. In this case, the minimum heat capacity rate $(mc_p)_{\min}=(mc_p)_2$ and Eq. (3) can be expressed as

$$T_3 = T_8\varepsilon_h + T_2(1-\varepsilon_h) \tag{4}$$

With no external heat transfer or work input, the first law of thermodynamics requires that $H_3-H_2=H_8-H_9$. Pressure drop through the regenerator is neglected. Therefore, $P_3=P_2$ and $P_8=P_9$.

Fuel Vaporizer. HCCI engines operate with premixed air-fuel intake charge. Liquid wet ethanol (ethanol-in-water) fuel is evaporated in the vaporizer before reaching the engine. The vaporizer consists of a low-pressure injector, similar to those used in throttle-body or port injected gasoline engines. The low-pressure injector provides good mixing between the fuel and the hot incoming air so that the ethanol and water can fully evaporate in the vaporizer. A system such as this has demonstrated good performance in HCCI experiments [17]. The vaporizer is analyzed using the laws of conservation of energy and mass: $H_3+H_4=H_5$; $\dot{m}_{O_2,3}=\dot{m}_{O_2,5}$; $\dot{m}_{N_2,3}=\dot{m}_{N_2,5}$; $\dot{m}_{H_2O,4}=\dot{m}_{H_2O,5}$, and $\dot{m}_{etOH,4}=\dot{m}_{etOH,5}$, where $\dot{m}$ is the mass flow rate of the different species and the numbers indicate locations in Fig. 3.

HCCI engines are typically run at low equivalence ratios ($\phi \leqslant 0.5$) to dilute the mixture and avoid violent combustion that may damage the engine. In our case, the air-fuel mixture is stoichiometric because the water mixed with the ethanol provides all the needed dilution.

Homogeneous Change Compression Ignition Engine. The premixed ethanol-water-air mixture from the vaporizer flows in the HCCI engine. No liquid fuel is injected directly into the engine. The intake charge mixes with hot residual gases and is compressed by the piston. Compression heats up the charge, leading to ignition and combustion if the peak temperature is high enough.

Combustion in HCCI engines is a bulk autoignition process controlled by chemical kinetics [7] and can be accurately predicted with a homogeneous reactor model that assumes well-mixed temperature, pressure, and composition in the combustion chamber. The homogeneous reactor has a variable volume that changes with time according to the slider-crank equation [14]. Limitations of the homogeneous reactor model include overestimating peak cylinder pressure and NO_x emissions [7], and being unable to predict HC and CO emissions that originate in the crevices and boundary layer. Distributed chemical kinetic models [7] can produce high fidelity HCCI simulations. However, their high computational cost makes them impractical for system level evaluation of regimes of HCCI operation.

Our homogeneous reactor model uses CHEMKIN [18] to handle thermodynamic and chemical kinetic data, and predicts HCCI combustion with a detailed reaction mechanism for ethanol autoignition chemistry [19] and NO_x kinetics [20] that contains 75 species and 485 chemical reactions. The homogeneous reactor model includes a wall heat transfer model [21] that assumes uniform cylinder liner, piston, and head temperatures (430 K). The homogeneous reactor model for the HCCI engine is computationally efficient (running in a few seconds in today's computers), which is an important advantage when making the many runs necessary to identify regions of efficient engine operation. The homogeneous model is unable to predict combustion inefficiencies caused by a lack of resolution of combustion gases in the cooler regions of the combustion chamber (crevices and boundary layer) that do not react to completion. An empirical correlation, obtained from experimental results [22], is therefore used for combustion efficiency η_c:

$$\eta_c = 0.94 \quad \text{if } \theta_{\max} < 0$$
$$\eta_c = 0.94 - 0.00667\theta_{\max} \quad \text{if } \theta_{\max} \geqslant 0 \tag{5}$$

In Eq. (5), $\theta_{\max}$ is the crank angle in degrees for maximum heat release ($\theta_{\max}=0$ at top dead center (TDC) $\theta_{\max}>0$ after TDC).

Engine analysis starts with the calculation of the residual gas fraction, the small fraction of complete combustion products left over from the previous cycle. The charge composition can then be calculated from the composition of the mixture at the vaporizer outlet (Point 5 in Fig. 3) and the composition of the residual gases. There is no external exhaust gas recirculation (EGR) in this engine system model. The mixed temperature of the residual gases and the fresh charge is calculated by a standard procedure ([14], Chap. 5). At this point, all the engine conditions at the beginning of the compression stroke are known, and the homogeneous reactor engine model can be run through the compression-expansion strokes. When the homogeneous reactor simulation is concluded, exhaust temperature is determined using the temperature of the combustion products at the time of exhaust valve opening (given by the homogeneous reactor simulation) and a thermodynamic model for gas expansion into the exhaust [14]. Performance parameters, including indicated efficiency and indicated power, are calculated by integrating the time-dependent thermodynamic data (pressure, temperature, and composition) for the engine cycle. Engine friction is calculated with an analytical procedure [23], and it is subtracted from the indicated power to calculate brake output power.

Catalytic Converter. While HCCI engines produce very little NO_x, they do require an oxidizing catalyst to control hydrocarbon and carbon monoxide emissions. Exhaust gases are hot enough that a diesel engine oxidizing catalyst (for example, Pd-loaded $SiO_2-Al_2O_3$ [24]) can burn the hydrocarbons and carbon monoxide that are not burned in the engine. The composition and temperature of the outlet gases are calculated from mass and enthalpy balances assuming complete combustion of HC and CO in the catalyst.

Analysis Methodology

In this paper, we optimize the energy balance for ethanol manufacture and utilization by minimizing the level of distillation required for successful and efficient operation in a HCCI engine. Considering that fermentation processes can efficiently produce ethanol at 12% by volume in water [5], it would be ideal to run the HCCI engine on 12% ethanol-water mixtures, with no distillation at all. However, this is quite unlikely. According to Fig. 4, the minimum ethanol concentration that can generate enough heat to evaporate the fuel and the water mixed with it is 11% by volume. Therefore, the minimum concentration of ethanol that can be burned in the HCCI engine cannot be lower than 11%, and it is likely to be much higher than this, as some of the chemical energy released by the ethanol combustion is converted to work in the engine and some is rejected with the exhaust gases.

Engine performance is calculated by incorporating all the system component equations described above into an iterative equation solver and a set of computational property tables [25]. The

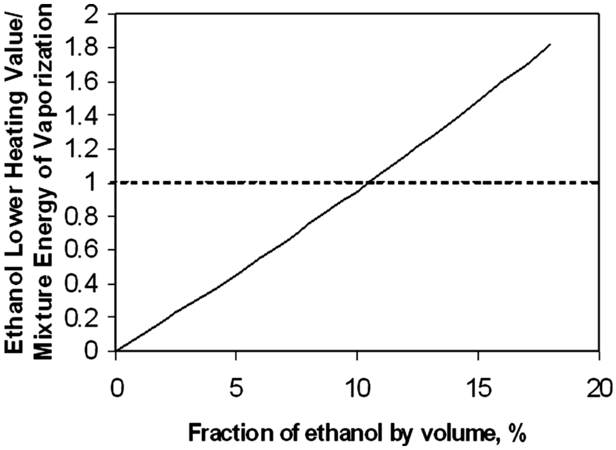

Fig. 4 Lower heating value divided by the latent heat of vaporization for mixtures of ethanol and water as a function of the ethanol volume concentration. The dotted horizontal line indicates the point at which the ethanol heating value is just enough to vaporize the mixture, corresponding to 11% ethanol in water by volume.

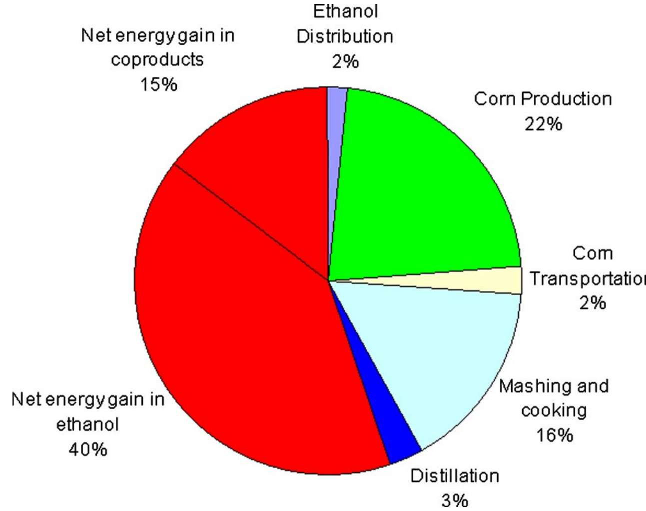

Fig. 5 Net energy balance for ethanol, considering production of a 35% ethanol in water by volume mixture appropriate as fuel for a HCCI engine. The figure shows wedges indicating energy consumption in all stages of ethanol production from corn, as a percent of the heating value of ethanol and coproducts. The energy that remains after accounting for all the energy consumption is the net energy gain, which has two components: net energy in the ethanol and net energy in the coproducts.

CHEMKIN-based HCCI engine combustion model is an external subroutine to the equation solver and is called when engine information is needed. The engine model is started with very low concentration of ethanol in water (15% by volume) and the ethanol concentration is gradually increased until efficient engine combustion is obtained, as predicted by the homogeneous reactor HCCI engine model.

Results

System model simulations are first conducted with 15% ethanol-in-water fuel supply, but we find that the water content is too high to sustain HCCI operation because components are too cool to achieve the needed energy balance. Gradually increasing the ethanol concentration, we find that the minimum fraction of ethanol in water necessary for efficient HCCI operation is 35% by liquid volume (14.3% by mole).

Figure 3 shows the thermodynamic conditions at all points in the HCCI engine system using 35% ethanol in water (by volume) as a fuel. The compressor delivers air at 300 kPa and 444 K, followed by the regenerator, which raises the air temperature to 727 K. Next, liquid ethanol in water is injected into the vaporizer, where it evaporates and mixes with air. The evaporation process in the vaporizer produces a homogeneous mixture of ethanol, water vapor, and air at 300 kPa and 412 K, which then enters the HCCI engine. The ethanol-water-air mixture inducted into the cylinder heats up to 420 K as it mixes with residual gases within the cylinder. After combustion, exhaust gases enter the catalytic converter at 870 K and exit the catalytic converter at 916 K due to heat release from conversion of HC and CO that were not reacted in the engine combustion chamber. Gases from the catalytic converter (215 kPa and 916 K) flow into the turbine, generating power that drives the turbocharger compressor. After circulating through the turbine, the exhaust gases exchange heat with the intake air in the regenerator and then leave the system at ambient pressure and 562 K.

The engine system model predicts 240 kW brake engine power at 38.7% brake thermal efficiency for the wet ethanol HCCI engine. Emissions of NO_x are predicted at 1.6 ppm (parts per million), low enough to meet any existing or oncoming standards for stationary and transportation applications. The wet ethanol HCCI engine combines high efficiency and low emissions, with the additional advantage of considerably improving the energy balance for ethanol. The wet ethanol HCCI engine is more efficient than typical SI engines, which are limited to ~35% peak brake thermal efficiency due to the low compression ratio necessary to avoid knock [26]. Diesel engines are more efficient, but they have high NO_x emissions that limit their applicability to markets without strict emissions standards.

Now that our simulations show that a HCCI engine can operate efficiently with wet ethanol, we investigate how modest distillation to 35% ethanol in water by volume affects the overall energy balance of corn-based ethanol production and utilization. Figure 1 shows that the net energy balance of fully distilled and dehydrated ethanol (pure ethanol) is positive but small, with only 21% net energy gain, 15% of this coming from coproducts. Now, referencing Fig. 2, we determine that using ethanol in water at 35% volume fraction (14.3% mole fraction) considerably reduces the energy required for distillation and dehydration, from 37% to only 3% of the total energy in ethanol product output (ethanol and coproducts). Only a small amount of distillation is required, and there is no need for dehydration when using wet ethanol. Figure 5 shows an energy balance for wet ethanol production, updated from the energy balance for production of fully distilled and dehydrated ethanol shown in Fig. 1. Figure 5 shows that by utilizing ethanol in water at 35% by volume, the net energy gain for ethanol produced (neglecting coproducts) increases from 6% to 40%. Total net energy gain (including coproducts) increases from 21% to 55%. In other words, for 35% ethanol in water, the ratio of energy output to energy input is 2.22:1, where the energy ratio for fully distilled and dehydrated ethanol is 1.27:1.

Our analysis gives evidence that HCCI engines can run efficiently on wet ethanol fuel and that utilizing wet ethanol fuel in HCCI engines improves the energy balance of ethanol production. Wet ethanol utilization is a promising concept that merits more detailed analysis and experimental evaluation.

Conclusions

The HCCI engine can operate on ethanol-water mixtures (wet ethanol) with high concentration of water. Our model indicates that a HCCI engine can run on 35% ethanol in water by volume and achieve high efficiency (38.7%) and very low NO_x (1.6 ppm, low enough to meet any current or oncoming standards).

Operation of the HCCI engine with 35% ethanol in water by volume reduces the energy required for distillation from 23% to

3% of the overall energy of ethanol and coproducts. There is no need for dehydration when using wet ethanol, yielding an additional 14% energy savings. This represents a 34% energy gain relative to fully distilled and dehydrated ethanol.

The net energy balance for ethanol is considerably improved by the use of wet ethanol. For pure ethanol, the net energy gain is 21% and only 6% if no coproducts are considered. Using 35% ethanol in water by volume increases the net energy gain to 55%, and 40% without considering coproducts. The ratio of energy output to energy input for 35% ethanol in water by volume is 2.22:1, compared with 1.26:1 for pure ethanol.

This analysis shows that the merits of the wet ethanol concept support conducting further analysis and experiments to show practical utilization of wet ethanol in a HCCI engine, and to show this as a path for improving the energy balance of ethanol, contributing to climate stabilization and improving energy security.

Acknowledgment

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Nomenclature

c_p = specific heat at constant pressure
c_v = specific heat at constant volume
H = enthalpy
$\dot{m}$ = mass flow rate
P = pressure
T = temperature
W = power
ε = heat exchanger effectiveness
ϕ = equivalence ratio
γ = specific heat ratio, c_p/c_v
η_c = combustion efficiency
η_p = polytropic efficiency

Subscripts

1–9 = locations in engine system diagram (Fig. 3)
c = compressor
t = turbine

References

[1] Pimentel, D., 2001, "The Limits of Biomass Energy," *Encyclopedia of Physical Science and Technology*, 3rd. ed., Academic, New York, Vol. 2, pp. 159–171.
[2] Shapouri, H., Duffield, J. A., and Graboski, M. S., 1995, "Estimating the Net Energy Balance of Corn Ethanol," USDA Economic Research Service Report No. AER-721, Washington, D.C.
[3] Shapouri, H., Duffield, J. A., and Wang, M., 2003, "The Energy Balance of Corn Ethanol Revisited," Trans. ASAE, **46**(4), pp. 959–968.
[4] Wyman, C. E., 1999, "Sterilization of Fermentation Vessels by Ethanol/Water Mixtures," US Patent 5,868,997.
[5] Ladisch, M. R., and Dyck, K., 1979, "Dehydration of Ethanol: New Approach Gives Positive Energy Balance," Science, **205**, pp. 878–900.
[6] Epping, K., Aceves, S. M., Bechtold, R. L., and Dec, J. E., 2002, "The Potential of HCCI Combustion for High Efficiency and Low Emissions," SAE Paper No. 2002-01-1923.
[7] Aceves, S. M., Flowers, D. L., Westbrook, C. K., Pitz, W., Smith, J. R., Dibble, R. W., Christensen, M., and Johansson, B., 2000, "A Multi-Zone Model for Prediction of HCCI Combustion and Emissions," SAE Paper No. 2000-01-0327.
[8] Sharke, P., 2000, "Otto or Not, Here It Comes," Mech. Eng. (Am. Soc. Mech. Eng.), **122**(6), pp. 62–66.
[9] Wolters, P., Salber, W., Geiger, J., Duesmann, M., and Dilthey, J., 2003, "Controlled Auto Ignition Combustion Process With an Electromechanical Valve Train," SAE Paper No. 2003-01-0032.
[10] Ohyama, Y., 2003, "Simultaneous Control of Air/Fuel Ratio and Intake, Exhaust Valve Timing for HCCI Operation," SAE Paper No. 2003-01-1084.
[11] Allen, J., and Law, D., 2002, "Variable Valve Actuated Controlled Auto-Ignition: Speed Load Maps and Strategic Regimes of Operation," SAE Paper No. 2002-01-0422.
[12] Koopmans, L., Strom, H., Lundgren, S., Backlund, O., and Denbratt, I., 2003, "Demonstrating a SI-HCCI-SI Mode Change on a Volvo 5-Cylinder Electronic Valve Control Engine," SAE Paper No. 2003-01-0753.
[13] Martinez-Frias, J., Aceves, S. M., Flowers, D., Smith, J. R., and Dibble, R., 2000, "HCCI Engine Control by Thermal Management," SAE Paper No. 2000-01-2869.
[14] Heywood, J. B., 1988, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York.
[15] Flowers, D., Martinez-Frias, J., Espinosa-Loza, F., Killingsworth, N., Aceves, S. M., Dibble, R., Krstic, M., and Bining, A., 2005, "Development and Testing of a 6-Cylinder HCCI Engine for Distributed Generation," *Proceedings of 2005 Fall Technical Conference ASME International Combustion Engine Division*, Long Beach, CA, Paper No. ICEF2005-1342.
[16] Wilson, D. G., 1993, *The Design of High-Efficiency Turbomachinery and Gas Turbines*, The MIT Press, Cambridge.
[17] Dec, J. E., and Sjöberg, M., 2003, "A Parametric Study of HCCI Combustion: The Sources of Emissions at Low Loads and the Effects of GDI Fuel Injection," SAE Paper No. 2003-01-0752.
[18] Kee, R. J., Rupley, F. M., Meeks, E., and Miller, J. A., 1996, "CHEMKIN III: A FORTRAN Chemical Kinetics Package for the Analysis of Gas-Phase Chemical and Plasma Kinetics," Sandia National Laboratories Report No. SAND96-8216, Livermore, CA.
[19] Marinov, N. M., 1999, "A Detailed Chemical Kinetic Model for High Temperature Ethanol Oxidation," Int. J. Chem. Kinet., **31**, pp. 183–220.
[20] Frenklach, M., Wang, H., Goldenberg, M., Smith, G. P., Golden, D. M., Bowman, C. T., Hanson, R. K., Gardiner, W. C., and Lissianski, V., 1995, "GRI-Mech: An Optimized Detailed Chemical Reaction Mechanism for Methane Combustion," GRI Topical Report No. GRI-95/0058.
[21] Woschni, G., 1967, "Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in the Internal Combustion Engine," SAE Paper No. 670931.
[22] Christensen, M., Johansson, B., Amneus, P., and Mauss, F., 1998, "Supercharged Homogeneous Charge Compression Ignition," SAE Paper No. 980787.
[23] Patton, K. J., Nitschke, R. G., and Heywood, J. B., 1989, "Development and Evaluation of a Friction Model for Spark-Ignition Engines," SAE Paper No. 890836.
[24] Ueno, H., Furutani, T., Nagami, T., Aono, N., Goshima, H., and Kasahara, K., 1998, "Development of Catalyst for Diesel Engine," SAE Paper No. 980195.
[25] Ho, C. Y., Liley, P. E., Makita, T., and Tanaka, Y., 1988, *Properties of Inorganic and Organic Fluids*, Cindas Data Series of Material Properties, Hemisphere, New York, Vol. V-1, Chap. 10.
[26] Aceves, S. M., Martinez-Frias, J., and Reistad, G. M., 2006, "Analysis of Homogeneous Charge Compression Ignition (HCCI) Engines for Cogeneration Applications," ASME J. Energy Resour. Technol., **128**, pp. 16–27.