Evaluation of state variable interface between the Activated Sludge Models and Anaerobic Digestion Model no 1

H. Yasui, K. Komatsu, R. Goel, Y. Y. Li and T. Noike

ABSTRACT

For plant wide modelling of wastewater treatment, it is necessary to develop a suitable state variables interface for integrating state of the art models of ASM and ADM1. ADM1 currently describes such an interface, however, its suitability needs to be experimentally evaluated. In this study, we characterised activated sludge under aerobic and anaerobic conditions to obtain representative state variables for both models. ASM state variables of X_S, X_H and X_I (as obtained from aerobic tests) and ADM1 state variables of X_C and X_I (as obtained from anaerobic tests) were then correlated to assess the suitability of current interface. Based on the seven datasets of this study and seven datasets from literatures, it was found that in general ASM state variables were well correlated to the state variables of ADM1. The ADM1 state variable of X_C could be correlated to the sum of state variables of X_S and X_H, while X_I in both the models showed direct correspondence. It was also observed that the degradation kinetics of X_C under anaerobic condition could be better described by individual degradation kinetics of X_S and X_H. Therefore, to establish a one to one correspondence between ASM and ADM1 state variables and better description of degradation kinetics in ADM1, replacing the composite variable of X_C by the state variables of X_S and X_H is recommended.

Key words | ADM1, ASM, hydrolysis, interface, respirometry, sludge composition

H. Yasui
Faculty of Environmental Engineering,
University of Kitakyusyu,
1-1 Hibikino, Wakamatsu-Ku,
Kitakyusyu, 808-0135,
Japan
E-mail: *hidenari-yasui@env.kitakyu-u.ac.jp*

K. Komatsu
Kurita Water Industries Ltd.,
1-1, Kwada-Gochoyama, Nogi,
Tochigi 329-0105,
Japan
E-mail: *kazuya.komatsu@kurita.co.jp*

R. Goel
Hydromantis Inc.,
1 James St South, Suite 1601,
Hamilton,
Ontario L8P 4R5,
Canada
E-mail: *goel@hydromantis.com*

Y. Y. Li
Department of Civil Engineering,
Tohoku University,
Aza-Aoba, Aramaki, Aoba-ku, Sendai,
Miyagi 980-8579,
Japan
E-mail: *yyli@epl1.civil.tohoku.ac.jp*

T. Noike
Advanced research Institute,
Nihon University, 4-2-1,
Kudan-kita, Chiyoda-ku,
Tokyo 102-0073,
Japan
E-mail: *noike@arish.nihon-u.ac.jp*

INTRODUCTION

Due to the introduction of Anaerobic Digestion Model no. 1 (ADM1, Batstone *et al.* 2002) and wide acceptance of Activated Sludge Models (ASMs, Henze *et al.* 2000), modelling of biological wastewater treatment plants has taken a new dimension leading to interest in development of plant wide models (Copp *et al.* 2003; Vanrolleghem *et al.* 2005; Volcke *et al.* 2006). One of the important requirements for plant wide modelling is that all of the unit processes in wastewater treatment plant are connected and simulated in an interdependent fashion. The issue of plant wide modelling would be trivial in case the models of all the unit processes are defined using a common set of state variables. However, the importance of this issue is appreciated as soon as it is realised that biological models do not necessarily share the same set of state variables. Differences in the set of state variable may arise due to the fact that 1) unit processes models are developed independently of each other, 2) the state variable important in one process may be

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redundant or less important in other unit process, or 3) available research data support only a particular set of state variables. Comparison of ASM and ADM1 reveals the differences in the state variables sets of the two models. Since ADM1 is consistently referred to ASMs throughout its development, the difference in state variable set is mainly due to the reasons of 2) and 3). Recognising the importance of state variable interface between ASM and ADM1, an interface is proposed in ADM1, however, its validity still needs to be experimentally supported.

Since organic substrate from activated sludge process to anaerobic digestion is mainly particulate in nature, the interface of particulate state variables between ASM and ADM1 is of high importance. Results of recent study by Yasui *et al.* (2006) suggested that the biodegradable and non-biodegradable fraction as estimated by ASM models might be correlated to the corresponding fractions in ADM1. Ekama *et al.* (2007) using a wide set of data concluded that the non-biodegradable fraction (from wastewater and due to decay of biomass) in activated sludge also remained non-biodegradable form under anaerobic condition. In this study we further evaluate the relationship between particulate state variables of ASM and ADM1 using new experimental datasets collected over different seasons. The study also proposes a modified ADM1 model structure complete with suitable kinetics and stoichiometric details.

MATERIAL AND METHODS

Apparatus for respirometry

Curves of methane production rate (MPR) and oxygen uptake rate (OUR) were obtained using batch respirometer supplied by Challenging Systems Inc., USA (AER-8). Temperature of the incubation vessel and the sensing device were maintained at 35 ± 0.2°C in a temperature-controlled incubator. For collecting MPR, a small scrubber consisting of caustic material was set between the incubation vessel and the sensing device to absorb CO_2 from the headspace gas. The data regarding methane gas production was logged at every two-hour interval in the computer. For identifying organic fractions in aerobic conditions, the respirometer was switched to aerobic mode. The consumed oxygen by microorganisms was equivalently supplied to the vessel kept at same temperature of 35°C as those in anaerobic tests. The measured OUR was analysed according to Copp *et al.* (2002) to identify ASM state variables.

Sludge samples

Seven activated sludge samples were taken from return line of a secondary settling tank of conventional activated sludge wwtp (Tohkamachi WWTP, Japan) operated with about 4–5 days of sludge retention time. The samples were collected at regular interval of 3–5 weeks during the period of June/2006 to February/2007. An additional sample was also collected from a different WWTP (Kitami WWTP, Japan) that was operated under similar condition to Tohkamachi wwtp. The samples were stored at 4°C for 1–2 days until the batch tests were conducted. Anaerobically digested sludge (seed sludge for anaerobic batch tests) was collected from the respective plants. The seed sludge was pre-incubated in the lab for 1–2 day to remove possible remaining biodegradable fractions that might lead to any background MPR. The activated sludge samples were washed twice using buffer solution ($NaHCO_3$:872 mg/l, K_2HPO_4:80 mg/l, KH_2PO_4 80 mg/l, pH = 7.5) of salt concentration comparable to anaerobic supernatant. The washed samples were then transferred to incubation vessels of 1,000 ml working volume. For anaerobic tests, adequate amount of pre-incubated anaerobic seed sludge and buffer solution were added to the washed activated sludge. The headspace was purged with nitrogen gas before sealing the incubation vessels. Through preliminary experiments, F/M ratios were set at below 0.45 (COD/COD) to avoid any significant VFA accumulation during the test period. A blank test ($F/M = 0$) was also conducted without addition of activated sludge to obtain MPR for endogenous respiration. For collecting respirograms under aerobic condition, buffer solution was added to the washed activated sludge samples. ATU in concentration of 15 mg/l was added to suppress oxygen consumption due to nitrification.

RESULTS AND DISCUSSION

Anaerobic and aerobic degradation curves

As shown in Figure 1, curve shape of the respirograms under anaerobic condition was substantially similar to that

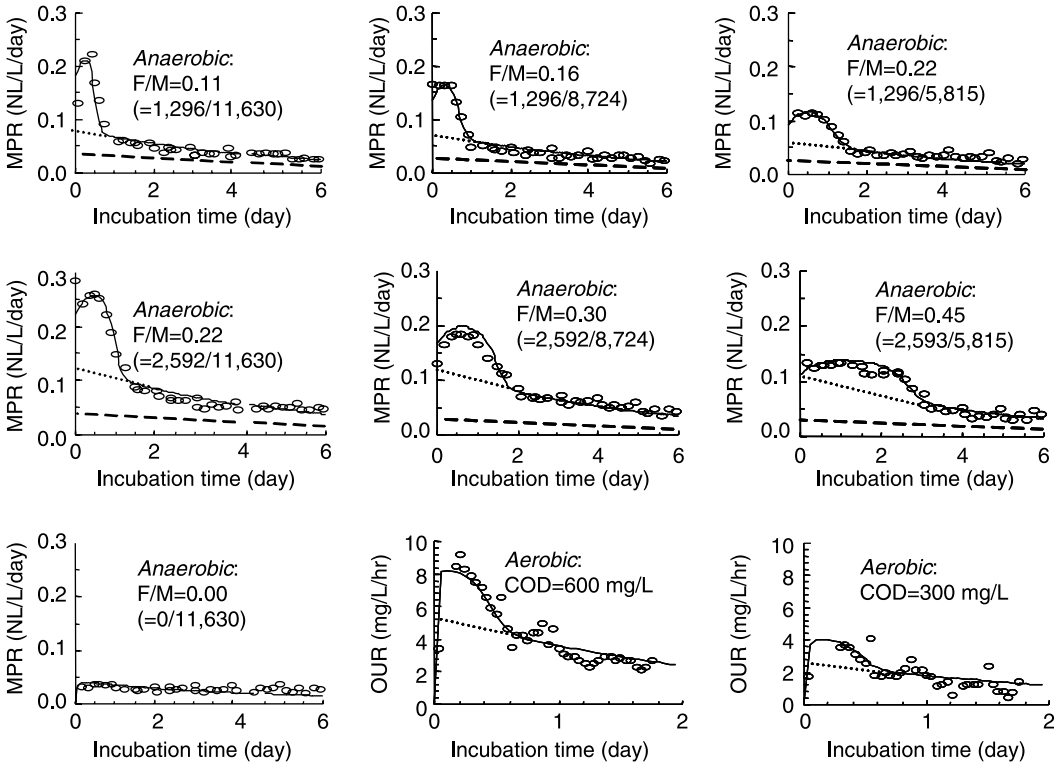

Figure 1 | Respirograms in anaerobic and aerobic condition in dataset of Kitami wwtp (–-: Baseline of seed sludge; …: Boundary between X_S and X_H; F/M ratio in COD basis).

under aerobic condition. In both conditions, higher initial degradation rate for initial 1–2 days (1st stage) were followed by mildly reducing lower degradation rates (2nd stage). This type of degradation curve is typical for degradation of mixed two substrates with fast and slow degradation kinetics. Since all the tests were carried out without any soluble degradable COD, the first stage initial high MPR (OUR) was thought to be due to hydrolysable particulate substrate fraction. In ASM, this substrate fraction is classified as X_S, while in ADM1 it is included in X_C. The second stage degradation curve was very typical of endogenous respiration (decay) of heterotrophic biomass. This degradable fraction corresponds to X_H in ASM and is a part of X_C in ADM1. Based on these observations, simplified model structures for aerobic and anaerobic digestion were prepared to simulate the observed simulation profiles in Tables 1 and 2 respectively.

The model for aerobic digestion of activated sludge was based on ASM1 and shows only the relevant modelled components where processes of hydrolysis of X_S, growth of heterotrophic biomass X_H and decay of X_H were considered. Concept of biomass death-regeneration was used for substrate recycling as in ASM1. In the anaerobic digestion model, seven processes were used. According to the anaerobic digestion model structure, X_S was assumed to be hydrolysed by X_H and X_{acid} (acidifier biomass) producing soluble substrate S_F (fermentable substrate). X_H was considered to decay anaerobically resulting in production of X_S and X_I. Other processes were prepared to describe growth /decay of X_{acid} and X_M (methanogens). The details of processes regarding individual intermediate soluble components typical in anaerobic digestion were skipped as they were not rate limiting. It shall be noted that to establish one to one correspondence between ASM and ADM1 models, state variables of X_S, X_H and X_I are common to both the models.

Table 1 | Aerobic digestion of activated sludge organics

Component → /Process ↓	X_S	X_H	S_F	X_I	Rate expression
Hydrolysis of X_S	−1		1		Contois type
Generation of X_H		1	$-1/Y_H$		Monod type
Decay of X_H *		−1	$1-f_I$	f_I	First order type

Table 2 | Anaerobic digestion of activated sludge organics

Component → /Process ↓	X_S	X_H	S_F*	S_{ac}†	X_{acid}‡	X_M§	X_I	Rate expression
Hydrolysis of X_S by X_H	-1		1					Contois type‖
Hydrolysis of X_S by X_{acid}	-1		1					Contois type¶
Decay of X_H		-1	$1-f_I$				f_I	First order type
Growth of X_{acid}			$-1/Y_{acid}$	$1/Y_{acid}-1$	1			Monod type
Growth of methanogens				$-1/Y_M$		1		Monod type
Decay of X_{acid}	$1-f_I$				-1		f_I	First order type
Decay of methanogens	$1-f_I$					-1	f_I	First order type

*S_F, Fermentable substrate (sum of S_{su}, S_{aa}, S_{fa}, S_{va}, S_{bu}, S_{pro}).
†S_{ac}, Substrate for methanogens (sum of S_{ac} *and* S_{h2}).
‡X_{acid}, Acidogens in AD sludge (sum of X_{su}, X_{aa}, X_{fa}, X_{c4}, X_{pro}).
§X_M, Methanogens in AD sludge (sum of X_{ac}, X_{h2}).
‖rate $= \eta_{an}\, k_H \times (aX_S/(K_X \times X_H + aX_S) \times X_H)$, $a = X_H/(X_H + X_{acid})$ (applied anaerobic hydrolysis reduction factor η_{an} of 0.07 under AD condition (Yasui *et al.* (2006)).
¶rate $= k_H \times ((1-a)X_S/(K_X \times X_{acid} + (1-a)X_S) \times X_{acid})$, $(1-a) = X_{acid}/(X_H + X_{acid})$.

Simulation studies for state variable interface evaluation

To use the above model structures for simulating the aerobic and anaerobic digestion of activated sludge, information regarding stoichiometric coefficients of Y_H, f_I, Y_{acid} (overall yield in acidogenesis stage) and Y_M (overall yield in methanogenesis stage) was necessary. As these coefficients have much influence in determining the values of X_S, X_H and X_I, representative values of these coefficients were required. Under aerobic condition, ASM1 recommends the value of coefficients of Y_H and f_I, which are almost constant at 0.67 and 0.08 respectively. The values of stoichiometric coefficients of Y_{acid} and Y_M, on the other hand, are substrate specific and literature values show larger variation. For example, ADM1 suggests value of Y_{acid} on carbohydrates from 0.01 to 0.17; Y_{acid} on amino acids from 0.058 to 0.16; Y_M on acetate from 0.014 to 0.076 and Y_M on hydrogen from 0.014 to 0.183. In this situation, representative values of Y_{acid} and Y_M were theoretically estimated using the principles of thermodynamics (Heijnen & van Dijken 1992).

The aerobic decay process could be expressed as Equation (1) where $(1+h)$ was equal to a reciprocal yield constant for regeneration of 1 unit biomass. By inputting corresponding values of standard Gibbs energy listed in Appendix I into the equation, the required Gibbs energy for 1 unit of biomass synthesis ($h\Delta G$) under aerobic condition was calculated to be 236.34 kJ/C-mol$_{Biomass}$ ($\because h = 0.49$). Since the required energy for synthesis was thought to be comparable under both aerobic and anaerobic condition (Heijnen & van Dijken 1992), by inputting the 236.34 kJ/C-mol$_{Biomass}$. to $h\Delta G$ in Equation (2) for anaerobic condition where ΔG was introduced to be 28.23 kJ/C-mol$_{Biomass}$ under reasonable H_2 partial pressure at 10^{-4} bar, $h = 8.37$ was obtained and thus Y_{acid} could be estimated to be 0.107.

$$(1+h)C_nH_xO_yN_z - h(aH^+ + bHCO_3^- + cH_2O + zNH_4^+ + dO_2 + \Delta G) - C_nH_xO_yN_z = 0 \quad (1)$$

where $(1+h) = Y_H^{-1} = 0.67^{-1}$, biomass formulation $= CH_{1.8}O_{0.5}N_{0.2}$ $(n=1,\ x=1.8,\ y=0.5,\ z=0.2)$, $a = (n-z) = 0.8$, $b = n$, $c = (-2n+x-3z)/2 = -0.4$,

Table 3 | Values of kinetic coefficients for Kitami WWTP and Tohkamachi WWTP

Parameter	Aerobic condition	Anaerobic condition
Decay rate of X_H, b_H	0.79 (0.50–1.2)	0.27 (0.15–0.40)
Maximum specific hydrolysis rate of X_S, k_h (day^{-1})	3.0 (1.2–5.0)	2.4 (0.4–6.0)
Half-saturation coefficient for hydrolysis of X_S, K_X (−)	0.071 (0.035–0.20)	0.071 (0.035–0.20)

Values in round brackets: minimum & maximum observed in the tests.

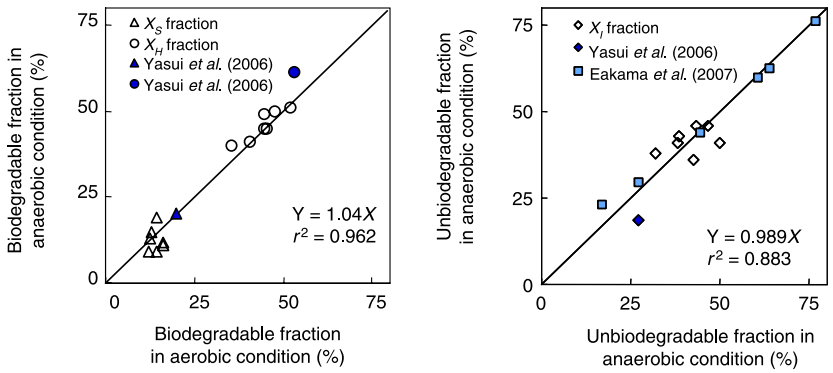

Figure 2 | Comparison of X_H, X_S, X_I ratios between aerobic and anaerobic conditions (●,▲,◆,■: Replotted from Yasui *et al.* (2006) and Ekama *et al.* (2007) by modified stoichiometry).

$d = (-4n - x + 2y + 3z)/4 = -1.05$, ΔG = released Gibbs energy (at standard condition) = 472.75 kJ/C-mol$_{\text{Biomass}}$.

$$(1+h)C_nH_xO_yN_z - h(aH^+ + bHCO_3^- + cH_2O + zNH_4^+ + df_{ac}C_2H_3O_2^- + d(1-f_{ac})H_2) + \Delta G) - C_nH_xO_yN_z = 0 \quad (2)$$

where, $(1+h) = Y_{\text{acid}}^{-1}$, biomass formulation = $CH_{1.8}O_{0.5}N_{0.2}$ ($n = 1$, $x = 1.8$, $y = 0.5$, $z = 0.2$), $a = \{(-2n - x + 2y - 3z)f_{ac} + 2n - 3z\}/(3f_{ac} + 1) = 0.41$, $b = \{(-n - x + 2y + 3z)f_{ac} - 3n + y\}/(3f_{ac} + 1) = 0.21$, $c = \{(-n + 2x - y - 6z)f_{ac} - 3n + y\}/(3f_{ac} + 1) = -0.92$, $d = (4n + x - 2y - 3z)/(6f_{ac} + 2) = 0.92$, $f_{ac} = 0.43$ (obtained from proportional mapping of "COD flow chart" in ADM1 (section 1.2), assuming biomass chemical composition: carbohydrates ≈12%, protein ≈76%, lipids ≈12% in COD basis), ΔG = released Gibbs energy (at $[H_2] = 10^{-4}$ bar) = 28.23 kJ/C-mol$_{\text{Biomass}}$ (introduced from ΔG at standard condition (15.90 kJ/C-mol$_{\text{Biomass}}$) − RT × 2.303 log $[H_2]^{d(1-\text{fac})}$).

The value of Y_M was calculated using an empirical equation estimating required Gibbs energy for growth of biomass from monomer compounds (hydrogen: $h\Delta G \cong 1{,}000$ kJ/C-mol$_{\text{Biomass}}$; acetate: $h\Delta G = 200 + 18(6 - C)^{1.8} + \exp[\{(3.8 - \gamma)^2\}^{0.16} \times (3.6 + 0.4C)] = 432$ kJ/C-mol$_{\text{Biomass}}$) proposed by Heijnen (1999). Where $C = 4$: number of carbon atoms in acetate, $\gamma = 2$: degree of reduction of carbon in acetate. Thus yield constant of acetoclastic methanogen $Y_{\text{Mac}} = 0.035$ gCOD/gCOD and that of hydrogen-utilising methanogen $Y_{\text{Mh2}} = 0.068$ gCOD/gCOD were obtained respectively. Based on the internal stoichiometric parameter f_{ac} of 0.43 derived from chemical composition of biomass, overall Y_M of 0.054 ($= 0.035 \times 43\% + 0.068 \times 57\%$) was used in this study.

Using these values of the stoichiometric coefficients, simulation of aerobic and anaerobic digestion was conducted (Figure 1). The calculated X_S, X_H and X_I fractions under aerobic and anaerobic conditions are summarised in Figure 1. Figure 2 also includes previous dataset of Yasui *et al.* (2006) and Ekama *et al.* (2007) for comparison. For datasets of Yasui *et al.* (2006), the estimated values of X_H and X_S were plotted slightly above the $Y = X$ line while X_I plots below. This was because a different set of stoichiometric constants ($Y_{\text{acid}} = 0.08$, $Y_M = 0$ and $f_I = 0.2$) was used in their study. For datasets from Ekama *et al.* (2007), X_I were almost plotted on $Y = X$ line as their used set of stoichiometric constants ($Y_{\text{acid}} = 0.113$, $Y_M = 0$ and $f_I = 0.08$) were almost identical to that used in this study. Although some data plots slightly scattered, in general it appeared that there was reasonable correspondence between the state variable of X_H, X_S and X_I under aerobic and anaerobic conditions. The estimated values of non-biodegradable fraction in present study also showed some seasonal variation (Figure 3). The observed variation in the value was about ± 15%. As the operational conditions at

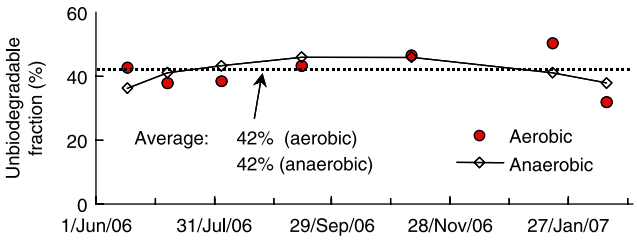

Figure 3 | Seasonal variation of unbiodegradable fraction in Tohkamachi WWTP.

the WWTP did not change, the observed change may be attributed to the change in the raw wastewater characteristics.

The kinetic values obtained from parameter-fitting of MPR and OUR are summarised in Table 3. It was observed that anaerobic decay rate (b_H) of X_H was always significantly lower than that observed under aerobic condition. The average anaerobic decay rate was estimated to be 0.27 day^{-1} (s.e. = 0.09) which was almost three times lower than the estimated aerobic decay rate of 0.79 day^{-1} (s.e. = 0.29). Although the reason of the reduction of b_H is not clear, it is speculated that reduced requirement of maintenance energy under anaerobic condition might be one of possible reasons. On the other hand, comparable kinetic values of k_h and K_X for degradation of X_S were obtained between anaerobic and aerobic condition. Rather than aerobic/anaerobic condition, seasonal variation seemed to affect the parameter values more significantly. However the kinetics of X_S would not give much impact on process performance in both AS and AD system because degradation rate of X_S was much higher than decay rate of X_H as observed through the batch tests. In practical condition, apart from X_I, the remaining degradable solid fraction in anaerobic digestion tank was considered to be mostly X_H, X_{acid} and X_M fractions.

CONCLUSION

Particulate state variable interface between ASM and ADM1 was evaluated based on OUR and MPR data from batch experiments. From the results, following three conclusions were obtained. The most prominent finding in the study was that the structure of anaerobic solid degradation of municipal activated sludge was comparable to that under aerobic condition. This means that the set of ASM state variables (X_S, X_H and X_I) can be used directly as interface between ASM and ADM1.

(1) The ASM state variables of X_S, X_H and X_I (as obtained from aerobic tests) and ADM1 state variables of X_C and X_I (as obtained from anaerobic tests) were well correlated.
(2) The degradation curve of activated sludge under aerobic and anaerobic conditions were quite similar and hence degradation kinetics under anaerobic condition could be described better by considering degradation of individual components of X_S and X_H rather than the composite variable of X_C.
(3) The anaerobic degradation of X_S could be modelled with Contois-type kinetics while X_H was modelled with first-order kinetics.

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Appendix I | List of Gibbs energy in standard condition

Species	Gibbs energy (kJ/mol)	Species	Gibbs energy (kJ/mol)
Biomass ($CH_{1.8}O_{0.5}N_{0.2}$)	−67.00	H^+	−39.87
H_2O	−237.18	$C_2H_3O_2^-$ (acetate)	−369.41
HCO_3^-	−586.85	CH_4 (methane)	−50.75
NH_4^+	−79.37	Elements (H_2, O_2, etc.)	0