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## Estimation of thermodynamic properties of hydrogen isotopes and <sup>2</sup> modeling of hydrogen isotope systems using Aspen Plus simulator

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#### A B S T R A C T

Physical properties of hydrogen isotopes, hydrogen (H2), hydrogen-deuterium (HD), hydrogen-tritium (HT), deuterium  $(D_2)$ , deuterium-tritium (DT), and tritium  $(T_2)$  were estimated through vapor pressure prediction, and validated by steady-state simulation of ITER isotope separation system (ISS). Peng– Robinson (PR) equation of state with Twu alpha function was selected for modelling which showed favorable prediction from the experimental vapor pressures of each hydrogen isotopes. The steady-state simulation of ITER ISS using Aspen Plus consists of four distillation columns and seven equilibrium reactors with four purified products:  $D_2$ ,  $T_2$ , HD, and DT. Converged solution from simulation produced potential scenario for actual ITER ISS process.

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### <sup>6</sup> Introduction

<sup>7</sup> For the practical production of fusion energy, seven entities, <sup>8</sup> South Korea, the United States, European Union, China, Russia, <sup>9</sup> Japan, and India, have gathered for the international nuclear fusion<br><sup>10</sup> experiment as a joint development project in progress. The  $10$  experiment as a joint development project in progress. The  $11$  experimental Boardor (TEP) project 11 International Thermonuclear Experimental Reactor (ITER) project<br>12 **International Photoscopy of the read from plasma physics** to  $12$  implies about achieving the road from plasma physics to  $13$  acceleration of revelops from a cover in which the word "itse" also <sup>13</sup> production of nuclear fusion power, in which the word "iter" also  $14$  means "way" in Latin. [Fig.](#page-1-0) 1 is a conceptual diagram showing the  $15$  represents the conceptual other components <sup>15</sup> ITER tritium fuel cycle. The gas fuel with several other components<br><sup>16</sup> including tritium is fed to a tekemak's terms chamber which  $^{16}$  including tritium is fed to a tokamak's torus chamber which<br> $^{17}$  consists of separation/purification/prequest, sustan of compo  $^{17}$  consists of separation/purification/recovery system of compo-<br> $^{18}$  ponts and then mixed again with the emitted gas Tekamak uses <sup>18</sup> nents, and then mixed again with the emitted gas. Tokamak uses<br><sup>19</sup> strong magnetic field to confine plasma into a stable flow of plasma 19 strong magnetic field to confine plasma into a stable flow of plasma<br>20  $\frac{20}{10}$  current in a doput-shaped vacuum chamber. The tokamak torus <sup>20</sup> current in a donut-shaped vacuum chamber. The tokamak torus  $\frac{21}{\pi}$  chamber is surrounded by magnetic field coils and transformers 21 chamber is surrounded by magnetic field coils and transformers.<br>22 Muclear fusion is generated by injecting ass inside the vacuumed <sup>22</sup> Nuclear fusion is generated by injecting gas inside the vacuumed  $\frac{23}{100}$  to the bight  $^{23}$  torus, heating by magnetic and electric field to form high-<br> $^{24}$  tomparature plasma and adding microwaves to further increase <sup>24</sup> temperature plasma, and adding microwaves to further increase<br><sup>25</sup> the temperature and squeeze the plasma. Tritium which is <sup>25</sup> the temperature and squeeze the plasma. Tritium, which is<br><sup>26</sup> introduced into a torus is released combined with other gases introduced into a torus, is released combined with other gases

Q2 \* Corresponding author. E-mail addresses: [jhcho@kongju.ac.kr,](mailto:jhcho@kongju.ac.kr) [pronjh1217@naver.com](mailto:pronjh1217@naver.com) (J. Cho). containing hydrogen isotopes from nuclear fusion reaction and  $^{27}$ <br>and form the terms  $^{28}$ proliferation process. The gas mixture discharged from the torus 28<br>processed to the tolerand outbourt processing (TED) to separate the 29 proceeds to the tokamak exhaust processing (TEP) to separate the 29<br>hydrogen isotopes with other impurities while the douterium and hydrogen isotopes with other impurities, while the deuterium and<br>tritium are congrated by cryogenic distillation in the isotope tritium are separated by cryogenic distillation in the isotope  $31$ <br>constrain cyclom (ISS). Then the constanted bydrogen isotopes  $32$ separation system (ISS). Then, the separated hydrogen isotopes  $32$ <br>through ISS are supplied for storage and delivery system (SDS). In  $33$ through ISS are supplied for storage and delivery system (SDS). In  $33$ <br>the water detritiation system (WDS), the remaining amount of  $34$ the water detritiation system (WDS), the remaining amount of  $34$ <br>deuterium and tritium are recovered and qualitative-quantitative deuterium and tritium are recovered, and qualitative–quantitative  $35$ <br>analysis is performed in the analysis system (ANS) In the fueling  $36$ analysis is performed in the analysis system (ANS). In the fueling  $36$ <br>system (ES) and noutral beam injector (NPI), the functions  $37$ system (FS) and neutral beam injector (NBI), the functions  $37$ <br>supplying the terms should be depended on the application of  $38$ supplying the torus should be depended on the application of  $38$ <br>the gas supplied from the SDS. The gases to be fed into the puckar  $39$ the gas supplied from the SDS. The gases to be fed into the nuclear  $\frac{39}{100}$ fusion reaction as fuel are  $T_2$ ,  $D_2$  and DT, and the gases to be  $\frac{40}{10}$ <br>injected in order to stan the nuclear fusion reaction are No. 4 m Ho injected in order to stop the nuclear fusion reaction are Ne, Ar, He,  $\frac{41}{2}$  $O_2$  and  $N_2$ , and the like [\[1](#page--1-0)–5]. This research proceeds with the study  $142$ <br>of the ISS process <sup>43</sup><br><sup>44</sup> of the ISS process.<br>ITER ISS is the system for purifying the desired component and

ITER ISS is the system for purifying the desired component and  $\frac{44}{100}$ <br>mosition using cryogenic distillation and the equilibrium  $\frac{45}{100}$ composition using cryogenic distillation and the equilibrium  $45$ <br>reaction in which gas mixture of hydrogen isotones from TFP  $46$ reaction in which gas mixture of hydrogen isotopes from TEP  $46$ <br>and WDS are fed [6.7]. On the other hand, since cryogenic  $47$ and WDS are fed [\[6,7\]](#page--1-0). On the other hand, since cryogenic  $47$ <br>distillation is used in the ISS there is a significant amount of  $48$ distillation is used in the ISS, there is a significant amount of  $\frac{48}{12}$ hydrogen isotopes being liquefied, and longer retention time of  $^{49}$ <br>tritium holdup during operation is the best present. Uslium 50 tritium holdup during operation is the best process. Helium  $50$ <br>refrigerator is used to aparate at low temperature of about 15, 20  $V = 51$ refrigerator is used to operate at low temperature of about  $15-20$  K.  $51$ <br>From TED and M/DS to ISS, the main compositions to be introduced  $52$ <sup>52</sup> From TEP and WDS to ISS, the main compositions to be introduced

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Fig. 1. Block diagram of ITER fuel cycle.

53 are the 6 hydrogen isotopes:  $H_2$ , HD, HT,  $D_2$ , DT, and  $T_2$ . In the ISS<br>54 process out of the six mixed gas D. DT and T, which are used as a 54 process, out of the six mixed gas,  $D_2$ , DT, and  $T_2$ , which are used as a raw material for ITER, should be purified with the desired composition. To produce the desired composition of  $D_1$ ,  $DT$  $^{56}$  compositions. To produce the desired composition of D<sub>2</sub>, DT,  $^{57}$  and T from ISS a tatal of four distillation activities as a set  $57$  and  $T_2$  from ISS, a total of four distillation columns and several  $58$  equilibrium governs (Faultinetes) should be installed by the  $^{58}$  equilibrium reactors (Equilibrator) should be installed. In the  $^{59}$ <sup>59</sup> equilibrium reactor, the following reversible reactions take place:<br> $\frac{60}{2}$  and  $\frac{1}{2}$  and  $\frac{1}{2$ 

60 2HD  $\leftrightarrow$  H<sub>2</sub> + D<sub>2</sub>, 2HT  $\leftrightarrow$  H<sub>2</sub> + T<sub>2</sub>, and 2DT  $\leftrightarrow$  D<sub>2</sub> + T<sub>2</sub>.<br>61 Table 1, adapted from Song et al. [\[8\]](#page--1-0), shows the equilibrium  $^{62}$  constant of isotopes based on temperature for each equilibrium<br> $^{63}$  constant constally these equilibrium reactions have clow reaction  $^{63}$  reaction. Generally, these equilibrium reactions have slow reaction<br> $^{64}$  rate at yery low temperature and fact reaction rate at ream  $^{64}$  rate at very low temperature and fast reaction rate at room<br> $^{65}$  temperature in terms of D, and T, generation. The desired <sup>65</sup> temperature in terms of  $D_2$  and  $T_2$  generation. The desired<br><sup>66</sup> melecular band form can load to a reaction when the cupplied  $^{66}$  molecular bond form can lead to a reaction when the supplied composition was set in the equilibrium reactor by optimizing the  $^{67}$  composition was set in the equilibrium reactor by optimizing the position of the equilibrium reactor [9]  $^{68}$  position of the equilibrium reactor [\[9\]](#page--1-0).<br> $^{69}$  FEB JSS presents 1906 a supersonic

 $^{69}$  ITER ISS process uses a cryogenic distillation and catalytic reaction from temperatures 14 to 30K Catalytic reaction takes  $70$  reaction from temperatures 14 to 30 K. Catalytic reaction takes<br> $71$  place in equilibrium in which the reactor should be installed in an  $71$  place in equilibrium in which the reactor should be installed in an  $72$  optimum position depending on the concentration profile of the <sup>72</sup> optimum position depending on the concentration profile of the  $^{73}$  column In addition with WDS linked to the ISS process a highly  $^{73}$  column. In addition, with WDS linked to the ISS process, a highly  $^{74}$  complex optimization technique will be required. Therefore, in  $^{74}$  complex optimization technique will be required. Therefore, in  $^{75}$  crds: to desire and optimize this presess, presess simulation  $^{75}$  order to design and optimize this process, process simulation<br> $^{76}$  chould be performed Housier, in Kerea, there are four to pens  $\frac{76}{77}$  should be performed. However, in Korea, there are few to none<br> $\frac{77}{77}$  examinations that have performed present simulation of the  $^{77}$  organizations that have performed process simulation of the cruceons is  $^{78}$  $^{78}$  cryogenic distillation process for the ITER ISS. One of the reasons is<br> $^{79}$  because domestic technology for the ISS process is still in the  $^{79}$  because domestic technology for the ISS process is still in the  $^{80}$  concent establishing phase and international technology also  $80$  concept establishing phase and international technology also  $81$  field to facilitate the tracking of related data which is critically  $\frac{81}{82}$  failed to facilitate the tracking of related data which is critically <sup>82</sup> low. Another reason is the lack of technology and the physical  $\frac{83}{2}$  are reason in the physical distillation are reason  $^{83}$  property data to perform the cryogenic distillation process  $^{84}$  cimulation. In this study the process unbusied properties for simulation. In this study, the necessary physical properties for







 $H_2$ , HD, HT, D<sub>2</sub>, DT, and T<sub>2</sub> components were obtained using the  $85$ equation of state which allows the simulation of the ISS process.

#### <sup>87</sup> Estimation of thermodynamic properties

### <sup>88</sup> Estimation of fixed properties of pure components

As shown in Table 2, the physical properties of the pure<br>monographs by the pure properties of  $\frac{1}{2}$  and  $\frac{90}{2}$ component for hydrogen isotopes, such as  $H_2$ , HD,  $D_2$ , HT, DT and  $T_1$  must be obtained in endea to estimate the above equilibrium  $10^{91}$  $T_2$ , must be obtained in order to estimate the phase equilibrium  $T_2$ , means time the equation of state such as Paps. Pobineen [10] 92 properties using the equation of state such as Peng–Robinson  $[10]$   $[92]$ <br>and Soave, Podlich Kwong [11]. However, from the compatibility  $[93]$ and Soave–Redlich–Kwong [\[11\]](#page--1-0). However, from the compatibility  $^{93}$ <br>of chamical process simulator such as Aspen Tosh Corporation's  $^{94}$ of chemical process simulator such as Aspen Tech Corporation's  $\frac{94}{25}$ Aspen Plus, Invensys' PRO/II with PROVISION, etc., only few  $^{95}$ <br>properties are built-in for H<sub>2</sub> HD and D<sub>2</sub> and no properties are  $^{96}$ properties are built-in for H<sub>2</sub>, HD and D<sub>2</sub>, and no properties are available for HT, DT, and T<sub>2</sub>. Thus, in this study, to estimate the 97 thermodus properties of H<sub>2</sub> HD<sub>D</sub>, HT<sub>2</sub> DT<sub>2</sub> and T<sub>2</sub> required thermodynamic properties of  $H_2$ , HD,  $D_2$ , HT, DT, and  $T_2$  required  $99$ <br>for the separation process, related experimental data were for the separation process, related experimental data were  $\frac{99}{200}$  collected which were used for regression applyis to obtain model  $\frac{100}{200}$ collected which were used for regression analysis to obtain model  $100$ <br>equation parameters, and finally to estimate thermodynamic  $101$ equation parameters, and, finally, to estimate thermodynamic  $101$ <br>neperties (Table 3)  $102$ properties ([Table](#page--1-0) 3). 102<br>The nure component properties for the six hydrogen isotopes 103

The pure component properties for the six hydrogen isotopes  $103$ <br>and an comprehensive study of eventimental data available in based on comprehensive study of experimental data available in  $104$ <br>literature [12, 14] are shown in Tables 2, and 4. The Gibbs free literature  $[12-14]$  $[12-14]$  are shown in [Tables](#page--1-0) 3 and 4. The Gibbs free  $105$ <br>concern for each of the component is presented in which the value energy for each of the component is presented in which the value  $106$ <br>for pure elements H, D, and T, are defined as zero (0) while the for pure elements,  $H_2$ ,  $D_2$  and  $T_2$ , are defined as zero (0), while the  $107$ <br>values for all the other compounds are defined by a specific value values for all the other compounds are defined by a specific value.  $108$ <br>The value of Gibbs free energy of formation  $\Delta C^{\circ}$  for the The value of Gibbs free energy of formation,  $\Delta G_{f,i}^{\circ}$ , for the  $110$  compounds are estimated from the standard Gibbs free energy  $110$  change free given absorbed received and change for a given chemical reaction. With these physical property  $111$ <br>unline the selection for the equilibrium reactor is serviced surface values, the calculation for the equilibrium reactor is carried out  $112$ <br>113  $(Table 4).$  $(Table 4).$  $(Table 4).$ 



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