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Advanced Tools for ITER Tritium Plant System Modeling & Design

J. M[a] Nougués,[a] J. A. Feliu,[a*] G. Campanyà,[a] E. Iraola,[a,b] L. Batet,[b] and L. Sedano[b,c]

[a]*INPROCESS Technology & Consulting Group, Gran Vía de Carles III, 86, 08028, Barcelona, Spain*
[b]*ETSEIB, Universitat Politècnica de Catalunya (UPC), Department of Physics, Diagonal 647, 08028, Barcelona, Spain*
[c]*FUS_ALIANZ Science, Engineering & Consulting, C/Nord 19, Atic, 43700, El Vendrell, Tarragona, Spain*

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Abstract — *Chemical plant system modeling experience based on the use of largely validated commercial modeling tools such as the Aspen HYSYS is adapted and exploited to develop numeric routines for unitary isotopic operations, including permeation, cold trapping, reversible absorption, and cryogenic distillation, for the ITER tritium plant systems. Model prediction capabilities and isotopic database inputs for first-principle models are discussed. Numeric implementation of the Aspen HYSYS routines are presented.*

Keywords — *Tritium migration, Aspen HYSYS, tritium unitary operations, tritium fuel cycle.*

Note — *Some figures may be in color only in the electronic version.*

I. INTRODUCTION

Tritium transfer modeling is a historical scientific milestone of nuclear fusion technology.[1] The current absence of experimental results at the required scale makes modeling a key tool for the design of existing and future facilities concerning tritium, such as the ITER experiment under construction (Ref. 2), the future DEMO (Ref. 3), or the CANDU nuclear power plants,[4] as well as any other hydrogen-related process plant where solute transport is especially important.

Tritium, in addition to being a radioactive isotope of hydrogen, is prone to permeate walls. When managing large inventories as ITER will (around 2 to 3 kg of tritium[5]), this becomes a major concern, and monitoring and control become crucial for licensing and safety.[6] This paper develops the first steps toward modeling and simulating tritium plant systems, starting with a general description of the needs and the choice of the Aspen HYSYS software in Sec. II, followed by the developments of unitary isotopic operations based on the ITER tritium plant, including permeation, cold trapping, reversible absorption, and cryogenic distillation, in Sec. III. Conclusions are presented in Sec. IV in terms of ongoing and further developments.

*E-mail: josepanton.feliu@inprocessgroup.com

II. ASPEN HYSYS AND ISOTOPIC DATABASES

A first-principle model (FPM) is a representation of reality based on well-established scientific laws only, avoiding assumptions as empiric correlations or parameter fitting. Applied to tritium, an FPM consists of the use of thermodynamic principles and is essential to accomplish predictive simulation.

Aspen HYSYS (Ref. 7) is a commercial software based on FPM that can represent unitary operations[a] mathematically in order to achieve a whole-plant model due to its capabilities of performing material and energy balances, liquid-vapor equilibrium, pressure drops, etc. Together with its customization possibilities through programming,[8] it is a great candidate to simulate new processes and to model nonexisting built-in operations such as permeation. Furthermore, the

[a] A unitary operation is the most fundamental step for a whole plant to yield the desired product. It involves a physical or chemical transformation such as, for example, filtration, evaporation, or permeation. Each unit operation follows the same physical laws and therefore may be used in all chemical industries.

flexible and plant-oriented environment of Aspen HYSYS also makes it prone to hold an entire fuel cycle simulation with the proper analysis for any kind of plant.

Unlike previous approaches to tritium transport modeling and fuel cycle design tools,[9–11] Aspen HYSYS offers a user-friendly graphical interface that allows a quick modeling experience. It has also been largely validated over the years by its thousands of users due to its highly extended use in industry, as well as in academia, for performing steady-state and dynamic simulations in process design and analysis.[12] Because of these reasons, Aspen HYSYS can substitute or complement other tools used in this field.

As an input, the FPM needs a database consisting of physico-chemical properties, liquid-gas transition data, kinetic and equilibrium reaction constants, and transport properties (e.g., diffusivity) of the isotopic forms of hydrogen gas (H_2, HD, D_2, HT, DT, T_2) and their oxidized forms, as isotopic properties are not present by default in the Aspen HYSYS's basis manager. Given that an open-access and standardized database does not exist to fit these requirements, a database was built in a previous report[13] by compiling data from literature, which is scarce for tritium,[14–16] and by computation of molecular collision potentials by means of Lenard-Jones potential,[17,18] through which any isotopic gas or mixture property can be deduced.

III. PREDICTIVE MODELING DEVELOPMENTS IN ASPEN HYSYS

The selected unitary operations concerning tritium, including (1) permeation, (2) cold trapping, (3) absorption/desorption, and (4) cryogenic distillation, have been implemented in Aspen HYSYS through direct implementation of built-in objects, Visual Basic–embedded programming, or a mixture of both in steady-state models. At the same time, programming can be performed by means of the creation of a brand new unit operation (called extension) or by adding or modifying behaviors to existing elements [through the so-called user defined variables (UDVs)]. Besides, simulations were checked in a previous report[13] against experimental results and/or analytical solutions.

III.A. Permeation in Aspen HYSYS

Isotope permeation is a singular unitary operation in nuclear fusion systems, taking into account the capability of hydrogen to permeate across materials. Permeation can happen willingly in separation systems such as the tokamak exhaust processing system of ITER (Ref. 19) where the objective is to separate hydrogen from other gases, and can occur unwittingly at any plant component where hydrogen is close to a wall. The expression of isotope permeation across membranes of Richardson law[20] has been directly programmed as a UDV for any built-in unitary operation, such as pipes (undesired permeation), and in a new and more sophisticated unitary operation representing the membrane operation (desired permeation). Figure 1 shows membrane unit operation in Aspen HYSYS.

III.B. Cold Trapping Process

The cold trapping process of elementary tritium forms can be assumed as a simple process consisting, in a first stage, of their oxidation into Q_2O forms (where Q stands for any atomic isotopic form of hydrogen, with the oxidized forms typically appearing as HTO and T_2O) and, in a second stage, in the freezing of these forms trapped at temperatures lower than −100ºC (Ref. 21).

Such characteristic ITER process has been implemented as several sequential unit operations in Aspen HYSYS using a reaction oxidation vessel plus an efficiency-imposed splitter whose performance can be made dependent on design parameters (volume, effective freezing surface, reaction kinetics, flow stream chemistry, etc.).

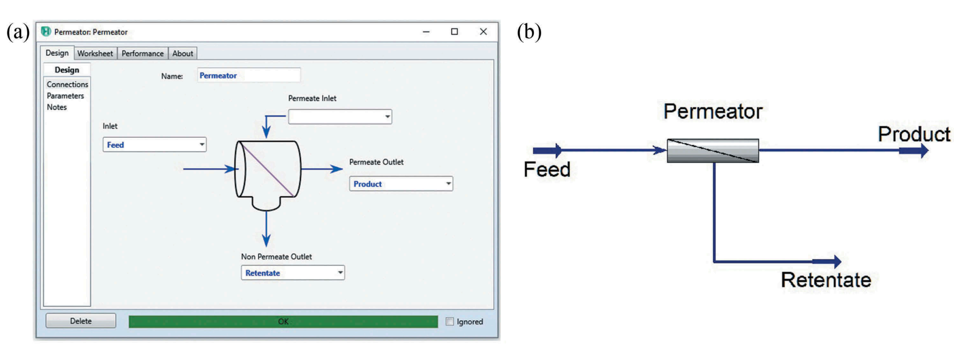

Fig. 1. (a) Permeator graphical user interface and (b) its depiction in a flow sheet layout in Aspen HYSYS.

III.C. Reversible Absorption/Desorption

Hydrogen isotope absorption/desorption processes are present all along the tritium plant systems in ITER, mainly at hydride beds in storage and delivery systems (SDSs) and long-term storage as a safe way of temporarily storing them due to the fact that they form hydrides with metals.[2] This is intended to occur in uranium beds as previously considered components such as ZrCo alloys are discarded because of a complex isotopic behavior called disproportioning.[22] Thus, the model built to represent hydride beds in Aspen HYSYS, whose flow sheet is shown in Fig. 2, is based on ideally reversible absorption and consists of three SDS lines in a bed and buffer layout.

III.D. Cryodistillation

Aspen HYSYS capabilities have been used in order to model the cryogenic distillation process. A distillation column built-in object (see Fig. 3) has been adapted to accomplish isotopic separation in steady state at the low-temperature range at which hydrogen boils up. Specifically, protium/deuterium separation has been successfully tested at impurity rates of 5%.

IV. CONCLUSIONS AND FURTHER WORK

The capabilities of the commercial process simulator Aspen HYSYS have been extended to satisfy the simulation needs of systems concerning tritium transport, such as ongoing fusion technology projects like ITER, the future DEMO project, or the CANDU reactors. These developments, which consist of modeling important operations in tritium transport such as permeation, cold trapping, absorption, and cryodistillation, support the

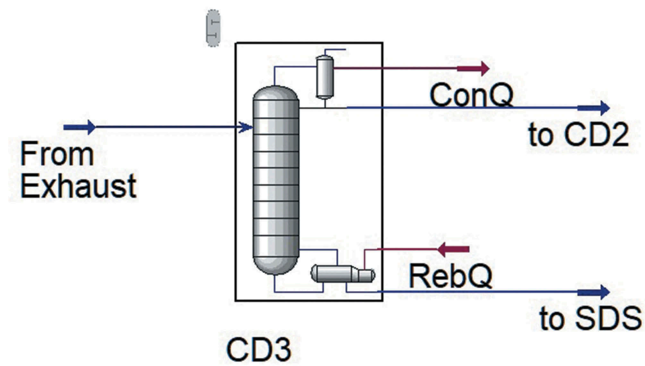

Fig. 3. Process flow diagram for single cryodistillation operation.

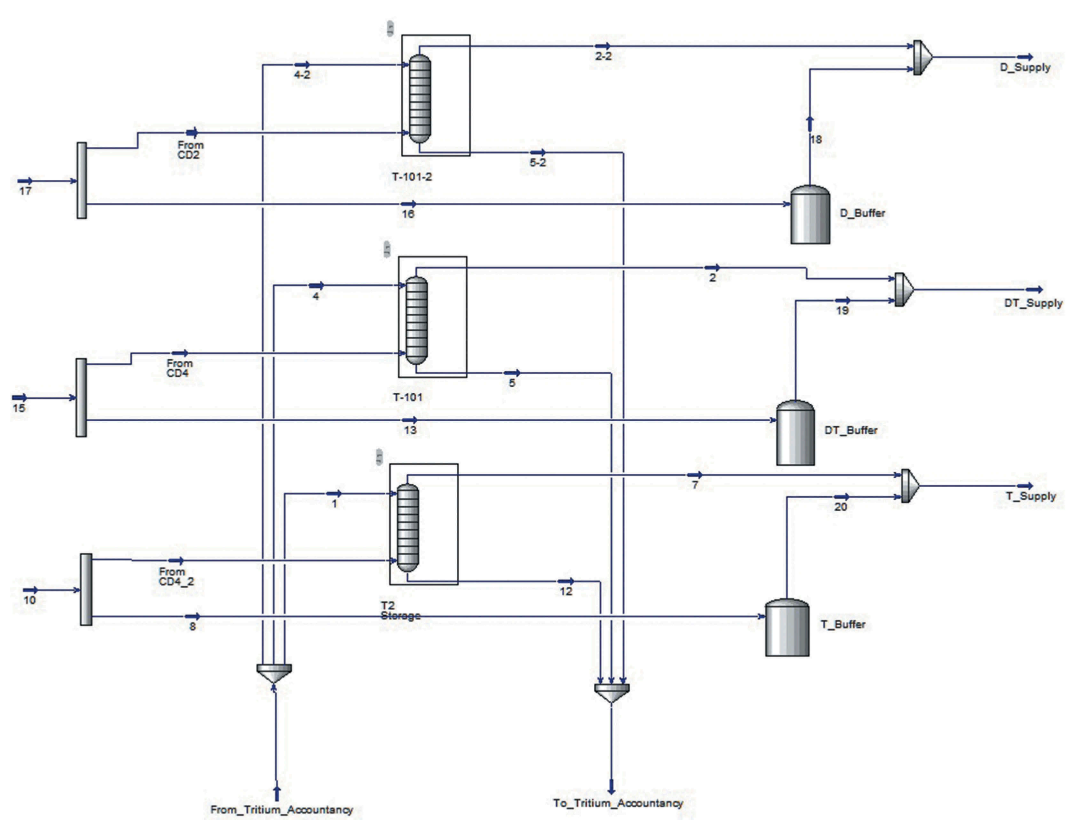

Fig. 2. Flow sheet of the absorption/desorption process implementation in Aspen HYSYS.

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conceptual design and detail engineering phase of the process design using steady-state simulation.

Further developments will focus on the expansion of current models to represent detailed larger systems, their validation, and the implementation of the extended calculation (unit operation, properties, and reactions) under dynamic mode. This last enhancement will enable the study of dynamic transients of the process and therefore deeper process analysis.

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ORCID

J. A. Feliu http://orcid.org/0000-0001-5163-9080

References

1. I. R. CRISTESCU et al., “Modeled Tritium Inventories Within the ITER Fuel Cycle Systems in Typical Fueling Scenarios,” *Fusion Sci. Technol.*, **52**, *3*, 659 (2007); https://doi.org/10.13182/FST07-A1564.
2. M. GLUGLA et al., “The ITER Tritium Systems,” *Fusion Eng. Des.*, **82**, *5–14*, 472 (2007); https://doi.org/10.1016/j.fusengdes.2007.02.025.
3. D. PERRAULT, “Nuclear Safety Aspects on the Road Towards Fusion Energy,” *Fusion Eng. Des.*, **146**, 130 (2018); https://doi.org/10.1016/j.fusengdes.2018.11.053.
4. J. M. MILLER, “Tritium Activities in Canada Supporting CANDU* Nuclear Power Reactors,” *Fusion Sci. Technol.*, **54**, *2*, 325 (2008); https://doi.org/10.13182/FST08-A1823.
5. I. R. CRISTESCU et al., “Tritium Inventories and Tritium Safety Design Principles for the Fuel Cycle of ITER,” *Nucl. Fusion*, **47**, *7*, S458 (2007); https://doi.org/10.1088/0029-5515/47/7/s08.
6. N. P. TAYLOR, “Safety and Licensing of Nuclear Facilities for Fusion,” *Proc. 2015 IEEE 26th Symposium on Fusion Eng. (SOFE)*, Austin, Texas, pp. 1–8 (2015); https://doi.org/10.1109/SOFE.2015.7482293.
7. “Aspen HYSYS,” ASPENTECH; https://www.aspentech.com/en/products/engineering/aspen-hysys (current as of Sep. 30, 2019).
8. *Aspen HYSYS Customization Guide*, ASPENTECH (2011).
9. A. BUSIGIN and P. GIERSZEWSKI, “CFTSIM-ITER Dynamic Fuel Cycle Model,” *Fusion Eng. Des.*, **39–40**, 909 (1998); https://doi.org/10.1016/S0920-3796(98)00222-1.
10. S. J. BRERETON, “Development of a Fusion Fuel Cycle Systems Code,” *Fusion Technol.*, **21**, *2P2*, 926 (1992); https://doi.org/10.13182/FST92-A29869.
11. I.-R. CRISTESCU et al., “ITER Dynamic Tritium Inventory Modeling Code,” *Fusion Sci. Technol.*, **48**, *1*, 343 (2005); https://doi.org/10.13182/FST05-A939.
12. C. SCHASCHKE, *A Dictionary of Chemical Engineering Oxford Quick Reference*, OUP Oxford (2014); https://doi.org/10.1093/acref/9780199651450.001.0001.
13. “Base de datos físicas, termofísicas y termoquímicas del hidrógeno e isótopos y de sus formas isotópicas oxidadas,” Internal Report, Inprocess Technology and Consulting Group, Barcelona, Spain (2016).
14. H. W. WOOLLEY, R. B. SCOTT, and F. G. BRICKWEDDE, “Compilation of Thermal Properties of Hydrogen in Its Various Isotopic and Ortho-Para Modifications,” *J. Res. Natl. Bur. Stand.*, **41**, *5*, 379 (1948); https://doi.org/10.6028/jres.041.037.
15. A. S. FRIEDMAN, D. WHITE, and H. L. JOHNSTON, “The Direct Determination of the Critical Temperature and Critical Pressure of Normal Deuterium. Vapor Pressures Between the Boiling and Critical Points,” *J. Am. Chem. Soc.*, **73**, *3*, 1310 (1951); https://doi.org/10.1021/ja01147a133.
16. E. R. GRILLY, “The Vapor Pressures of Hydrogen, Deuterium and Tritium up to Three Atmospheres,” *J. Am. Chem. Soc.*, **73**, *2*, 843 (1951); https://doi.org/10.1021/ja01146a103.
17. C. L. KONG, “Combining Rules for Intermolecular Potential Parameters. II. Rules for the Lennard-Jones (12-6) Potential and the Morse Potential,” *J. Chem. Phys.*, **59**, *5*, 2464 (1973); https://doi.org/10.1063/1.1680358.
18. H. K. SHIN, “Inelastic Molecular Collisions with a Lennard-Jones (12-6) Interaction Energy,” *J. Chem. Phys.*, **41**, *9*, 2864 (1964); https://doi.org/10.1063/1.1726367.
19. M. GLUGLA et al., “Recovery of Tritium from Different Sources by the ITER Tokamak Exhaust Processing System,” *Fusion Eng. Des.*, **61–62**, 569 (2002); https://doi.org/10.1016/S0920-3796(02)00250-8.
20. L. SEDANO, “Tritium Cycle Design for He-Cooled Blankets for DEMO,” Internal Report 1110, CIEMAT (2007).
21. N. BEKRIS et al., “Cold Trapping of Traces of Tritiated Water from the Helium Loops of a Fusion Breeder Blanket,” *Fusion Eng. Des.*, **58–59**, 423 (2001); https://doi.org/10.1016/S0920-3796(01)00477-X.
22. N. BEKRIS and M. SIRCH, “On the Mechanism of the Disproportionation of ZrCo Hydrides,” *Fusion Sci. Technol.*, **62**, *1*, 50 (2012); https://doi.org/10.13182/FST12-A14111.