Consistent analysis of deuteron interactions at low and medium energies

M. Avrigeanu and V. Avrigeanu
Horia Hulubei National Institute for Physics and Nuclear Engineering, P.O. Box MG-6, 077125 Bucharest-Magurele, Romania
E-mail: marilena.avrigeanu@nipe.ro

Abstract. An extended discussion of the deuteron-induced reactions concerning full parametrization procedure as well as consideration of the theoretical models associated to the deuteron interaction process is carried out. The key role of direct interactions, i.e., breakup, stripping and pick-up processes is stressed out by comparison of the available experimental data with theoretical and evaluation predictions.

1. Introduction
An update of the theoretical analysis of deuteron-nuclei interaction highly requested by on-going strategic research programs (ITER, IFMIF, SPIRAL2-NFS) [1] and medical investigations using accelerated deuterons has been considered since a decade ago within the FENDL-library project [2]. This update was motivated essentially by the specific noncompound processes that should be considered in the case of the incident deuterons, making them substantially different from other incident particles. Thus, the deuteron breakup (BU) is particularly quite important due to the large variety of reactions initiated by the breakup nucleons along the whole incident energy range. Otherwise, the deuteron interaction with low and medium mass target nuclei at incident energies below and around the Coulomb barrier proceeds largely through direct reaction (DR) mechanisms, stripping and pick-up, while pre-equilibrium emission (PE) and evaporation from fully equilibrated compound nucleus (CN) become important at higher energies [5].

More recently, full parametrization of the deuteron monitor reactions and therapeutic radionuclides-production cross sections have been recommended within Special Issues on Nuclear Reaction Data by Hermanne et al. [3], and Engle et al. [4]. Thus, genuine Padé fit of the available data has been involved at variance, however, with the FENDL [2] concern of improved theoretical analysis of the deuteron-induced reactions. Actually, Engle et al. [4] motivated the choice of the Padé fit, despite less predictive power and apart from nuclear modeling advance, by the deficiency in the theoretical description of the deuteron breakup. Therefore it seems appropriate a comparative analysis of empirical parametrization and microscopic studies within the experimental data and theoretical predictions leading to a final evaluation of deuteron data.

2. Additive reaction cross-section parametrization and model analysis
A particular case in this respect could be the interconnection of two valuable complementary experimental data sets of $^{231}\text{Pa}(d,3n)^{230}\text{U}$ and $^{231}\text{Pa}(p,2n)^{230}\text{U}$ [6] excitation functions, measured between [11.2 - 19.9 MeV] [6], and [10.6 - 23.8 MeV], respectively, which have been...
Figure 1. Comparison of the measured [6], latest TENDL-2017 [24] evaluation (dotted curve) and model calculation (solid curve) including the BF (dashed curve), and PE+CN contribution to $^{231}\text{Pa}(d,3n)^{230}\text{U}$ reaction cross sections calculated without (dash-dot-dotted) and with (dot-dashed) inclusion of the BU effect on $\sigma_R$.

analyzed separately also by Padé fit due to the assumed deficiency in the theoretical deuteron breakup description [4]. Actually, the particular value of the $^{231}\text{Pa}(p,2n)^{230}\text{U}$ reaction cross-section measurements [6] comes from the superposition of its incident–energy range and the breakup proton energies corresponding to the energy range of the reaction $^{231}\text{Pa}(d,3n)^{230}\text{U}$ [7].

We pointed out earlier [7, 8] the dominant role of the breakup mechanism in the interaction process of deuterons with Actinides targets at incident energies around Coulomb barrier. The proper handling of both breakup components – the elastic breakup (EB), in which the target nucleus stays in its ground state, and the inelastic breakup (BF), where one of the breakup nucleons interacts non-elastically with the target nucleus – leads to the description of the $^{231}\text{Pa}(d,3n)^{230}\text{U}$ excitation function shown in Fig. 1 [7].

On the whole, the leakage of the initial deuteron flux toward the breakup process reduces the total reaction cross section $\sigma_R$ that should be shared among different outgoing channels by a reduction factor $(1 - \sigma_{BU}/\sigma_R)$ [7, 8, 9, 10, 11], where $\sigma_{BU}$ is the total breakup cross section. This effect is shown in Fig. 1 for the $^{231}\text{Pa}(d,3n)^{230}\text{U}$ reaction comparing PE and CN mechanisms contribution to $(d,3n)$ reaction without (dash-dot-dotted curve) and with (dot-dashed curve) inclusion the correction for the incident flux leakage through the breakup [7]. On the other hand, the interaction with the target nucleus of a breakup proton enhances the $(d,3n)$ residual channel population through $(p,2n)$ reaction (Fig. 1) [7], stressing out the importance of their simultaneous analysis.

Concerning the deuteron monitor reactions described with Padé fit by Hermanne et al. [3], almost all of them have already been analyzed in the frame of BU, DR, PE and CN reaction mechanisms models [9, 10, 11]. These analyzes covered the whole experimental systematics of the deuteron induced reactions on the natural element target and its isotopes, making possible a reliable understanding of the interaction process. Confidence in the reaction cross-section predictions at energies where the measurements still not exist, aimed by the FENDL project, has thus been provided. An example of the complete analysis of the deuteron interaction with a target nucleus is given in the following.

3. Analysis of deuteron induced reactions on $^{55}\text{Mn}$ target nucleus

3.1. Direct Interactions

The specific noncompound processes, namely the direct interactions (DI) such us breakup and stripping and pick-up direct reactions, make deuteron-induced reactions substantially different from reactions with other incident particles. Actually, noticeable discrepancies between the measured activation data and theoretical model results follow mainly the disregard of the deuteron interaction process peculiarity [9, 10, 11].
3.1.1. Breakup. Our description of the deuteron breakup mechanism is based on the parametrization [12] of both the total breakup proton emission $\sigma_{BU}^p$ and EB cross sections, assuming equal inelastic-breakup cross sections for the breakup neutron and proton. The energy dependence of the deuteron total-reaction cross section $\sigma_R$, the total-breakup and $\sigma_{BU}^p$ cross sections, as well as the breakup components $\sigma_{EB}$ and $\sigma_{BF}^p$ for deuteron interactions with $^{55}$Mn target nucleus are compared in Fig. 2(a). The breakup excitation functions increase with deuteron-energy increasing, showing also the dominant role of the BF component.

On the whole, the enhancing effect of the breakup mechanism is important mainly for description the excitation functions for second and third chance emitted-particle channels [7, 8, 9, 10, 11]. The BF enhancements due to the BU protons and neutrons emitted during the deuteron interaction with $^{55}$Mn, through the $(p, x)$, and $(n, x)$ reactions populating various residual nuclei, are discussed in Sec. 4.

3.1.2. Direct reactions. The appropriate calculation of the DR stripping and pick-up mechanism contributions has been performed using the distorted-wave Born approximation (DWBA) formalism within the code FRESCO [13], with details given elsewhere [9, 10, 11]. Experimental angular distributions of particle emission in deuteron-induced DRs on $^{55}$Mn there are only for the $(d, p)$ stripping and $(d, t)$ pick-up reactions. Their suitable description (Figs. 3 and 4) has validated the correctness of the $(d, p)$ and $(d, t)$ excitation-function calculations shown in Fig. 2(b).

However, because of the missing data for $(d, n)$ stripping and $(d, \alpha)$ pick-up reactions, the sum $\sigma_{(d,p)} + \sigma_{(d,t)}$ stands only as a lower limit of the DR component shown also in Fig. 2(b). It has a significant maximum around $E_d \sim 7$ MeV mainly due to the $(d, p)$ strong stripping processes. It will be shown in Sec. 4 the major role of the stripping $(d, p)$ reactions to the activation cross sections of $^{56}$Mn residual nucleus, for deuteron interaction with $^{55}$Mn, as well as the exclusive contribution of $(d, t)$ pick-up process to population of $^{54}$Mn residual nucleus at the lowest incident energies, up to the thresholds of the $(d, nd)$ and $(d, 2np)$ reactions.

Finally, consideration of the reduction factor of the incident flux due to its absorption within BU as well as DR processes provides the correct deuteron total cross-section going towards
Figure 3. Comparison of measured (solid circles) [14] and calculated (solid curves) proton angular distributions of $^{55}$Mn($d,p)^{56}$Mn stripping transitions to states with excitation energies in MeV, at the incident energy of 7.5 MeV.

Figure 4. As Fig. 3 but for triton angular distributions [15] from $^{55}$Mn($d,t)^{54}$Mn pick-up reaction at the incident energy of 18 MeV.

PE+CN statistical decay of the excited system:

$$1 - \frac{\sigma_{BU} + \sigma_{(d,p)} + \sigma_{(d,t)}}{\sigma_R} = 1 - \frac{\sigma_{DI}}{\sigma_R}. \quad (1)$$

Its energy dependence is shown in Fig. 2 (c) at once with that corresponding to BU and DR reaction mechanisms, pointing out the important role of each one in the deuteron interaction process with $^{55}$Mn target nucleus.

3.2. Statistical emission

The PE and CN statistical processes contributions have been calculated using the TALYS-1.9 code [16] and the reduction factor of Eq. 1 in order to take into account the above-mentioned absorption of the deuteron flux into the DI processes.
Figure 5. Comparison of measured excitation functions [21, 22, 23], TENDL-2017 evaluated [24] (short-dashed curves), and calculated results (solid thick curves) of deuteron-induced reactions on $^{55}$Mn (see text).

The following input options of the TALYS-1.9 code have been used: (a) the OMPs of Koning-Delaroche [17], Daehnick et al. [18], Becchetti-Greenlees [19], and Avrigeanu et al. [20] for neutrons and protons, deuterons, tritons, and $\alpha$-particles, respectively, (b) the back-shifted Fermi gas (BSFG) formula for the nuclear level density, (c) no TALYS breakup contribution, since the above-mentioned BF enhancements is still under implementation in TALYS, and (d) the PE transition rates calculated by means of the corresponding OMP parameters.

4. Results and discussion

The detailed contributions of all involved reaction mechanisms, pointing out the strength of each one, may lead however to the well improved agreement of measured data and model calculation results with reference to the TENDL evaluated data (Fig. 5). The mark BU for the sum of various contributions to an activation cross section in Fig. 5 underlines the consideration of both breakup effects, i.e., the decrease of $\sigma_R$ due to the deuteron breakup, and the BF enhancement. Additional comments concern the reaction types and residual nuclei as follows.

4.1. The $^{55}$Mn($d$, $p$)$^{56}$Mn reaction

The analysis of the population of $^{56}$Mn residual nucleus through deuteron interaction with $^{55}$Mn represents actually a distinct test of the reaction model approach due to the dominant contribution of the ($d$, $p$) stripping mechanism. The comparative analysis of the reaction mechanism contributions involved in the $^{55}$Mn($d$, $p$)$^{56}$Mn reaction, shown in Fig. 5(a), points out the key role of the stripping. Thus, the PE+CN component is lower by more than one order of magnitude, while BF contribution brought by breakup neutrons through $^{55}$Mn($n$, $\gamma$)$^{56}$Mn reaction is practically negligible and not visible in this figure. The key role of the ($d$, $p$) stripping process has been pointed out also within previous analyzes of deuteron interaction with $^{51}$V, $^{50}$Cr, $^{58}$Fe, $^{64}$Ni, and $^{93}$Nb [9, 10] target nuclei.

4.2. The $^{55}$Mn($d$, $x$)$^{54}$Mn reaction

The analysis of the $^{55}$Mn($d$, $x$)$^{54}$Mn reaction, Fig. 5(b), is the most interesting one from the viewpoint of the variety of contributing reaction mechanisms. The residual nucleus $^{54}$Mn is populated entirely through the pick-up reaction ($d$, $t$) at incident energies lower than $\sim$11 MeV, i.e. below the thresholds for emission of more particles in ($d$, $nd$) and ($d$, $p2n$) reactions, with a PE+CN faster increase and a maximum around 29 MeV. Then, two inelastic-breakup enhancing contributions, through the $^{55}$Mn($n$, $2n$)$^{54}$Mn and $^{55}$Mn($p$, $n$)$^{54}$Mn reactions induced by breakup-nucleons, become dominant above 42 MeV. Altogether, the sum of the five reaction contributions succeeded to describe the measured $^{55}$Mn($d$, $pxn$)$^{54}$Mn excitation function. Moreover, the
underestimation of the lowest-energy data by the TENDL-2017 evaluation could be just the effect of a \((d,t)\) pick–up process overlooking as it was pointed out also in previous analysis of deuteron interaction with \(^{nat}\)Ni and \(^{93}\)Nb \([9, 10]\).

4.3. The \(^{55}\)Mn\((d,x)\)^{51}\)Cr reaction
Among possible reaction channels, \(^{55}\)Mn\((d,\alpha2n)\)^{51}\)Cr represents the main contribution to \(^{51}\)Cr population in the whole energy interval, as it is suggested by the data in Fig. 5(d). As shown within previous analyzes of deuterons interacting with Fe, Ni, and Cr target nuclei \([9, 10]\), the measured population of \(^{51}\)Cr residual nucleus is a cumulative process \([10]\), the \(EC\) decay of \(^{51}\)Mn residual nucleus to \(^{51}\)Cr being much shorter \((T_{1/2}=46.2\) min\) than the measurement time of the induced activity. However, the contribution brought by \(^{51}\)Mn decay should be considered negligible due to the higher thresholds of the reactions \((d,t3n)\) and \((d,p5n)\) populating it, of 36.8 MeV and 45.6 MeV, respectively. A suitable account of \(^{51}\)Cr excitation function has been obtained in this work taking into consideration the PE+CN statistical processes as well as the inelastic-breakup enhancement brought by breakup-nucleons interaction with \(^{55}\)Mn. The BF contribution becomes significant above the incident energy of 40 MeV, improving well the agreement of the measured data and model calculation.

4.4. The \(^{55}\)Mn\((d,x)\)^{52}\)gMn reaction
The accurate recent measurements of the excitation function of \(^{52}\)gMn activation \([22, 23]\) have nevertheless represented a must of a consistent and complete analysis of deuteron-activation of manganese. Population of \(^{52}\)gMn residual nucleus follows mainly the statistical PE+CN mechanisms [Fig. 5(c)], the BF enhancement due to breakup nucleons being weaker by at least two orders of magnitude. A sudden underestimation of these data appears below \(\sim 37\) MeV. On the other hand, this underestimation concerns an energy range below thresholds of possible reactions populating \(^{52}\)Mn, as 25.9 MeV for \(^{55}\)Mn\((d,t2n)\), 32.4 MeV for \(^{55}\)Mn\((d,d3n)\), and 34.7 MeV for \(^{55}\)Mn\((d,p4n)\).

At this point, it became of interest to take into account the fact that these excitation functions \([22, 23]\) were measured using targets consisted of a natural high purity \(Ni(2\%)-Mn(12\%)-Cu(86\%)\) alloy. In this respect, the authors found that only negligible corrections had to be introduced to their measured data derived for \(^{55}\)Mn.

Nevertheless, we have included in Fig. 5(c) the measured data \([25, 26]\) and calculated cross sections (dash-dotted curve) for \(^{52}\)gMn activation by deuterons on Ni but reduced with a correction factor 1/6 corresponding to the Ni/Mn relative amount within the target alloy. The comparison of the data for the two reactions is suggestive of a Ni contribution within the measurements for Mn at the incident energies below the lowest threshold of the above-mentioned reactions on \(^{55}\)Mn. This contribution becomes indeed negligible at higher energies as well as in the whole energy range and within two orders of magnitude for the other three reactions in Fig. 5. However, this contribution addition of Ni activation in the target alloy of Refs. \([22, 23]\) to the model results corresponding to \(^{55}\)Mn\((d,x)\)^{52}\)gMn reaction shown in Fig. 5(c) seems to describe well the measured data reported for \(^{52}\)gMn activation by deuterons on Mn. It is thus confirmed the suitable account of all available measured cross sections for deuteron activation of Mn by the present model approach.

5. Conclusions
A detailed theoretical treatment of each reaction mechanism has made possible a reliable understanding of the interaction as well as accurate values of the calculated deuteron activation cross sections.
The comparison of the experimental deuteron activation cross sections and present model calculations as well as the corresponding TENDL-2017 evaluation supports the detailed theoretical treatment of deuteron interactions, while the discrepancies between the measured data and this evaluation are the result of overlooking the inelastic breakup enhancement and less appropriate treatment of stripping and pick-up processes. This comparison particularly indicates the role of direct interactions to provide the suitable description of deuteron data.

The recently increased interest on the breakup theoretical analysis (e.g., [27] and Refs. therein) may lead eventually to the refinement of the deuteron breakup parametrization and increased accuracy of the deuteron activation cross section calculations.

The consistent theoretical frame of the deuteron interactions supported by advanced codes associated to the nuclear reactions mechanisms provides predictability in addition to the use of various-order genuine Padé approximations [3, 4] needed in applications.

Acknowledgments
Acknowledgments This work has been partly supported by Autoritatea Nationala pentru Cercetare Stiintifica (Project PN-19060102) and Euratom research and training program 2014-2018 and 2019-2020 under Grant Agreement No. 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

References
[1] www.iter.org, www.ifmif.org, www.ganil-spiral2.eu
[2] Fusion Evaluated Nuclear Data Library (FENDL) 3.0, https://www-nds.iaea.org/fendl3/
[3] A. Hermann et al. 2018 Nucl. Data Sheets 148, 338
[4] J.W. Engle et al. 2019 Nucl. Data Sheets 155, 56
[5] M. Avrigeanu and V. Avrigeanu 2015 Phys. Rev. C 92, 021601(R)
[6] A. Morgenstern et al. 2009 Phys. Rev. C 80, 054612; A. Morgenstern et al. 2008 Anal. Chem. 80, 8763
[7] M. Avrigeanu, V. Avrigeanu, and A. J. Koning 2012 Phys. Rev. C 85, 034603
[8] M. Avrigeanu and V. Avrigeanu 2016 J. Phys: Conf. Ser. 724, 012003; 2018 J. Phys: Conf. Ser. 1023, 012009; 2017 EPJ Web of Conferences 146, 012020
[9] E. Šimečková et al. 2018 Phys. Rev. C 98, 034606; A. Kreisel et al. 2019 Phys. Rev. C 99, 034611
[10] M. Avrigeanu et al. 2013 Phys. Rev. C 88, 014612; 2014 Phys. Rev. C 89, 044613; 2016 Phys. Rev. C 94, 014606; M. Avrigeanu and V. Avrigeanu 2014 Nucl. Data Sheets 118, 301
[11] P. Bém et al. 2009 Phys. Rev. C 79, 044610; E. Šimečková et al. 2011 Phys. Rev. C 84, 014605; I. Mador et al. 2018 Eur. Phys. J. A 54, 91
[12] M. Avrigeanu and V. Avrigeanu 2017 Phys. Rev. C 95, 024607; M. Avrigeanu and A. M. Moro 2010 Phys. Rev. C 82, 037601; M. Avrigeanu et al. 2009 Fusion Eng. Design 84, 418
[13] J. J. Thompson 1988 Comput. Phys. Rep. 7, 167; 2011 v. FRES 2.9
[14] J. R. Comfort 1969 Phys.Rev. 177, 1573
[15] T. Taylor and J. A. Cameron 1976 Nucl. Phys. A 257, 427
[16] A. J. Koning, S. Hilaire, and S. Goriely 2017 v. TALYS-1.9 http://www.talys.eu
[17] A. J. Koning and J. P. Delaroche 2003 Nucl. Phys. A 713, 231
[18] W. W. Daehnick, J. D. Childs, and Z. Vrcelj 1980 Phys. Rev. C 21, 2253
[19] F. D. Becchetti, Jr. and G. W. Greenlees 1969 John H. Wiliams Laboratory Annual Report 1969 (Minnesota Univ., Minneapolis p. 116; https://wwwosti.gov/servlets/purl/4908657/
[20] V. Avrigeanu, P. E. Hodgson, and M. Avrigeanu 1994 Phys. Rev. C 49, 2136
[21] Experimental Nuclear Reaction Data (EXFOR), https://www-nds.iaea.org/exfor/; J. L. Gilly et al. 1963 Phys.Rev. 131, 1727; N. Baron and B. L. Cohen 1963 Phys.Rev. 129, 2636; P. P. Coetzee and M. Peisach 1972 Radiochimica Acta 17, 1
[22] F. Ditroi et al. 2011 Nucl. Instr. and Meth. in Phys. Res. B 269, 1878
[23] Tarkányi et al. 2019 J. Radioanalytical and Nuclear Chemistry 320, 145
[24] A. J. Koning and D. Rochman, 2017 TENDL-2017: TALYS-based evaluated nuclear data library https://tendl.web.psi.ch/tendl_2017/tendl2017.html
[25] S. Takács et al. 2007 Nucl. Instr. and Meth. in Phys. Res. B 260, 495
[26] A. Hermann et al. 2013 Nucl. Instr. and Meth. in Phys. Res. B 299, 8
[27] G. Potel et al. 2017 Eur. Phys. J. A. 53, 178