Implementation of a GDH model in TALYS:
first results and perspective use

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Objectives

- to collect "all the best" in one popular code

- to extend the predictive power and the spectrum of application of the combination GDH+EQ by the use of Hauser-Feshbach model

- to take advantage of GDH combined with H-F model for nuclear data evaluation

GDH + H-F. Famous combinations

STAPRE-H95 M. Avrigeanu, V. Avrigeanu

EMPIRE 2.19 M. Herman, R. Capote, B. Carlson, P. Oblozinsky, M. Sin, A. Trkov, V. Zerkin

DDHMS module M. Chadwick

The planned improvement: B.V.Carlson, 2010

Karlsruhe Institute of Technology

The hybrid and GDH model

J.J.Griffin, 1966 : exciton model

G.D.Harp, J.M.Miller, B.J.Berne, 1968 : master-equation approach

M.Blann, 1971 : “hybrid” model

M.Blann, 1972 : “geometry dependent hybrid” model

Importance of nuclear density distribution on pre-equilibrium decay

M.Blann, H.K.Vonach, 1983 : modification and basic improvement of GDH

exciton level density, particle mean free path, initial exciton numbers etc.

J.Bisplinghoff, 1986 : critical analysis

Configuration mixing in pre-equilibrium reactions

hybrid model: zero intrinsic configuration mixing

exciton model: maximum mixing

1994 : cluster emission in nucleon induced reactions

d, t, He-3, α, Be-7: Exciton coalescence pick-up model (Sato, Iwamoto, Harada (1982,1983), knock-out model

M.Blann, 1996 : hybrid Monte Carlo simulation (HMS)

New precompound decay model

Karlsruhe Institute of Technology

2005 : improvement of pre-equilibrium cluster emission calculation in GDH

C.A.Soares Pompeia, B.V.Carlson, 2006 : comparative study of configuration mixing in pre-equilibrium reactions in exciton and hybrid models

No-mixing model (HMS) provides the more consistent description of pre-equilibrium reactions. Complete-mixing assumed in exciton model is not attained in the early reaction stages.

The GDH model

$$\frac{d\sigma}{d\varepsilon_x} = \pi \lambda\!\!\!^{-2} \sum_{l=0}^{\infty} (2l+1) T_l \sum_{n=n_0} {}_n X_x \frac{\omega(p-1,h,U)}{\omega(p,h,E)} \frac{\lambda_x^e}{\lambda_x^e + \lambda_x^+} \; g \; D_n$$

Emission rate

$$\lambda_x^e = \frac{(2S_x+1)\,\mu_x\,\varepsilon_x\,\sigma_x^{inv}(\varepsilon_x)}{\pi^2 \hbar^3 g_x}$$

Intranuclear transition rate

$$\lambda_x^+ = V \sigma_0(\varepsilon_x)\,\rho_l$$

ρ_l: $\; l\lambda\!\!\!^{-}$ to $(l+1)\lambda\!\!\!^{-}$

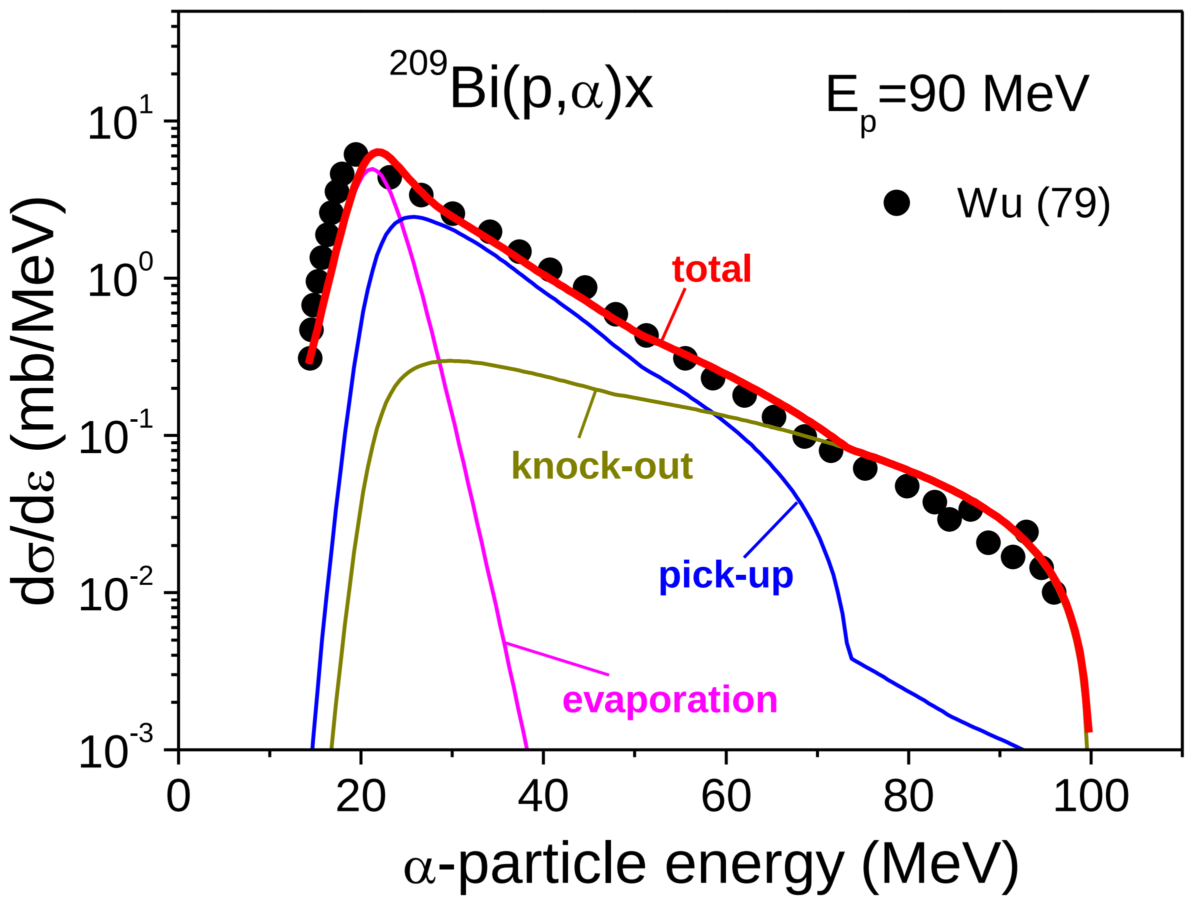
Precompound α-particle emission

$$\frac{d\sigma}{d\varepsilon_\alpha} = \frac{d\sigma^{pick-up}}{d\varepsilon_\alpha} + \frac{d\sigma^{knock-out}}{d\varepsilon_\alpha}$$

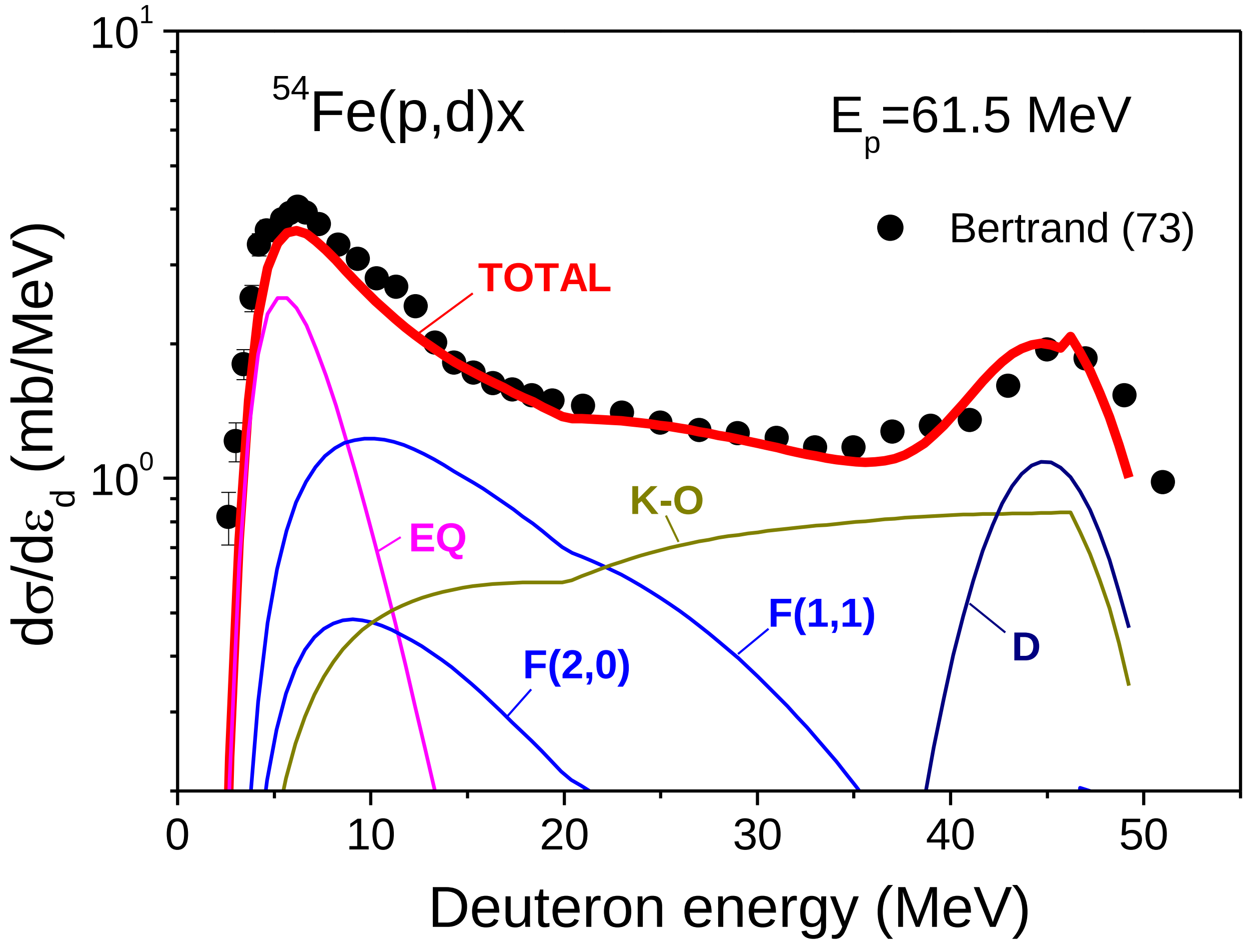
$$\frac{d\sigma^{pick-up}}{d\varepsilon_\alpha} = \sigma_{non} \sum_{n=n_0} \sum_{k+m=4} F_{k,m}(\varepsilon_\alpha) \frac{\omega(p-k,h,U)}{\cdot\ \omega(p,h,E)} \frac{\lambda^e_\alpha(\varepsilon_\alpha)}{\lambda^e_\alpha(\varepsilon_\alpha)+\lambda^+_x(\varepsilon_\alpha)} g_\alpha D_n$$

$$\frac{d\sigma^{knock-out}}{d\varepsilon_\alpha} = \sigma_{non} \sum_{n=n_0} \varphi_\alpha \frac{g}{g_\alpha\ p} \frac{\omega(p-1,h,U)}{\omega(p,h,E)} \frac{\lambda^e_\alpha(\varepsilon_\alpha)}{\lambda^e_\alpha(\varepsilon_\alpha)+\lambda^+_x(\varepsilon_\alpha)} g_\alpha D_n$$

Example of calculations with ALICE/ASH (FZK)



Example of calculations with ALICE/ASH (FZK)



GDH in TALYS

modified TALYS subroutines: 6

modified ALICE/ASH subroutines: 30

new subroutines: 7

GDH: mpreeqmode=5

various GDH options: subroutine gdhinput

last e-mail exchange with Arjan: 16.09.2009

last modifications: 17.11.2009, subroutine gdhfin

Comparison with basic TALYS calculations

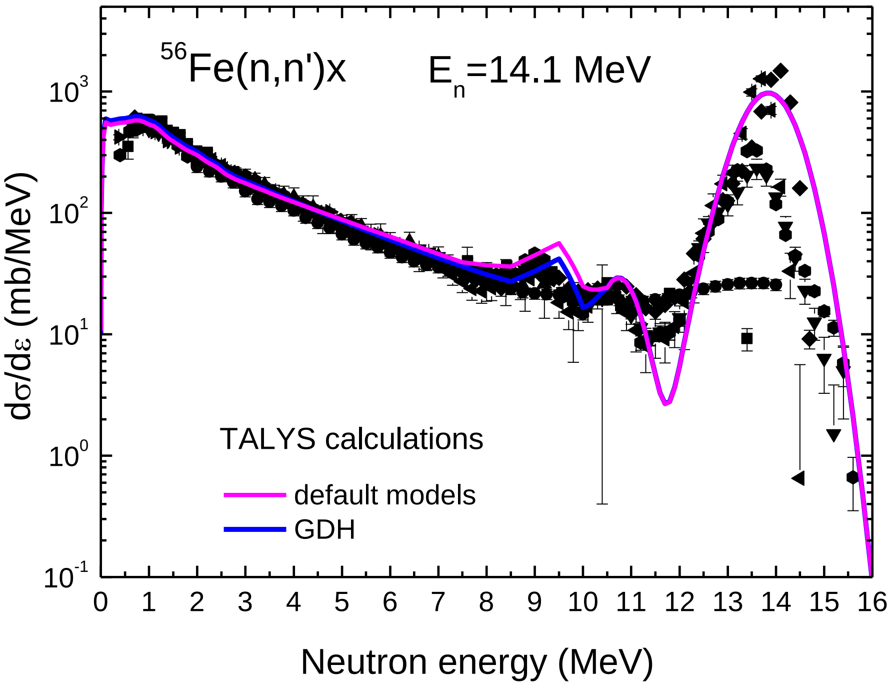
"default models" of TALYS

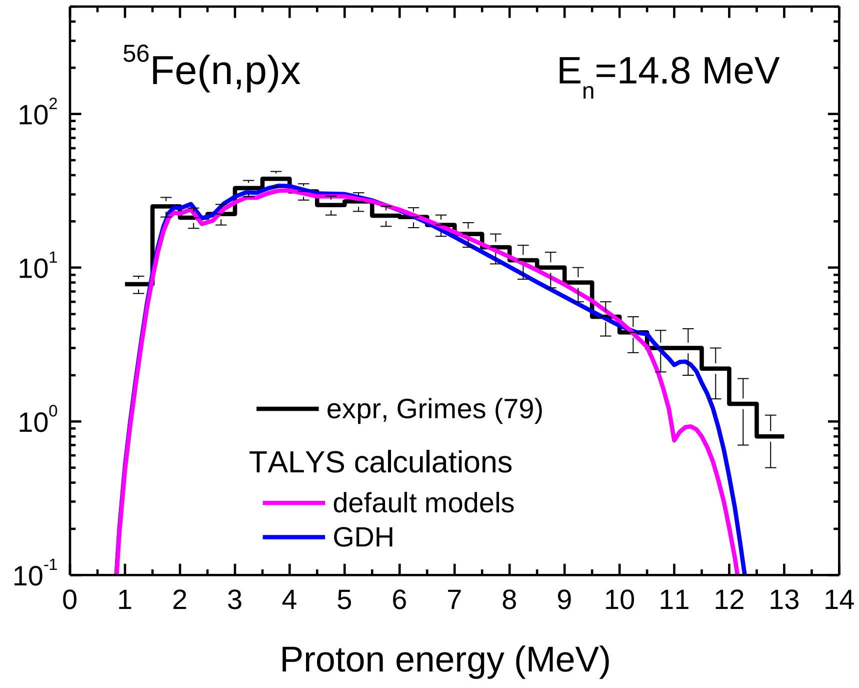
Pre-equilibrium exciton model: A.J.Koning, M.C.Duijvestijn, NP, 2004

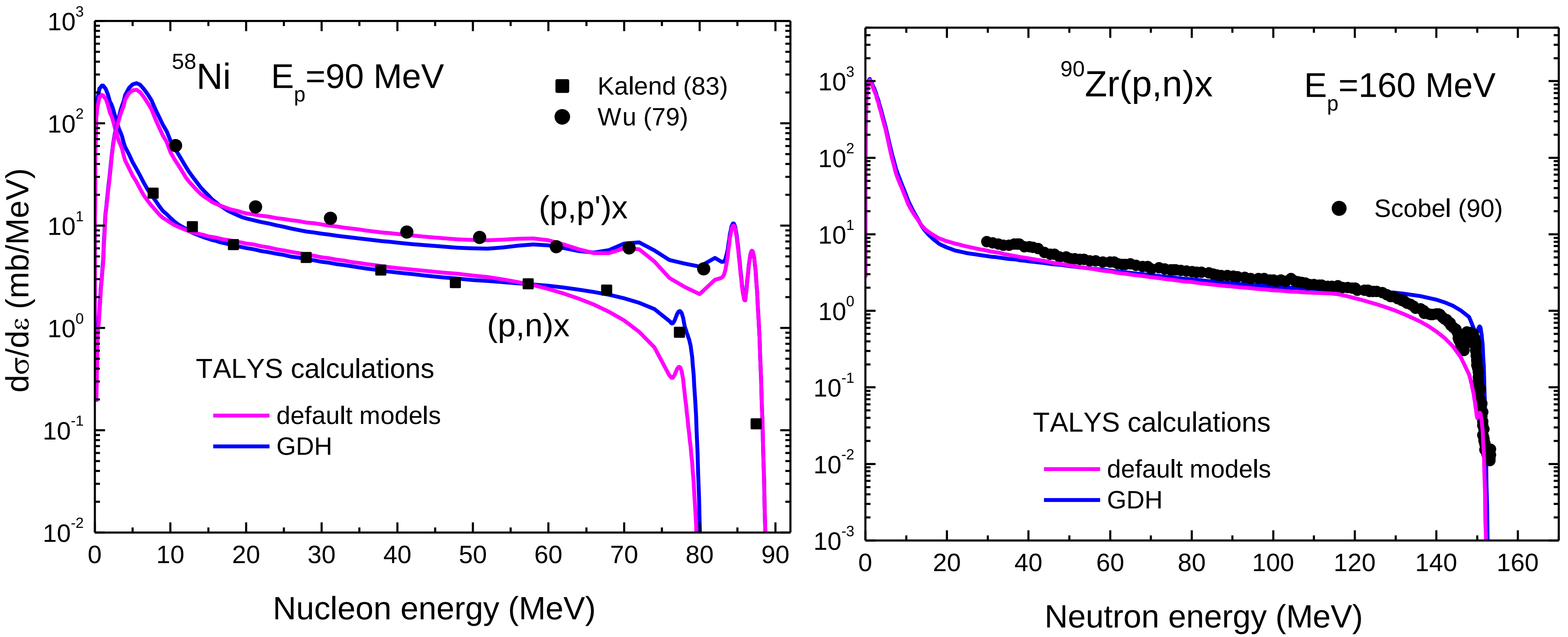
Complex particle emission: C.Kalbach, ZPA, 1977, PRC 2005

Nuclear level density: Gilbert-Cameron-Ignatyuk-Smirenkin-Tishin
A.J.Koning, S.Hilaire, M.C.Duijvestijn, 2007

Nucleon energy distributions

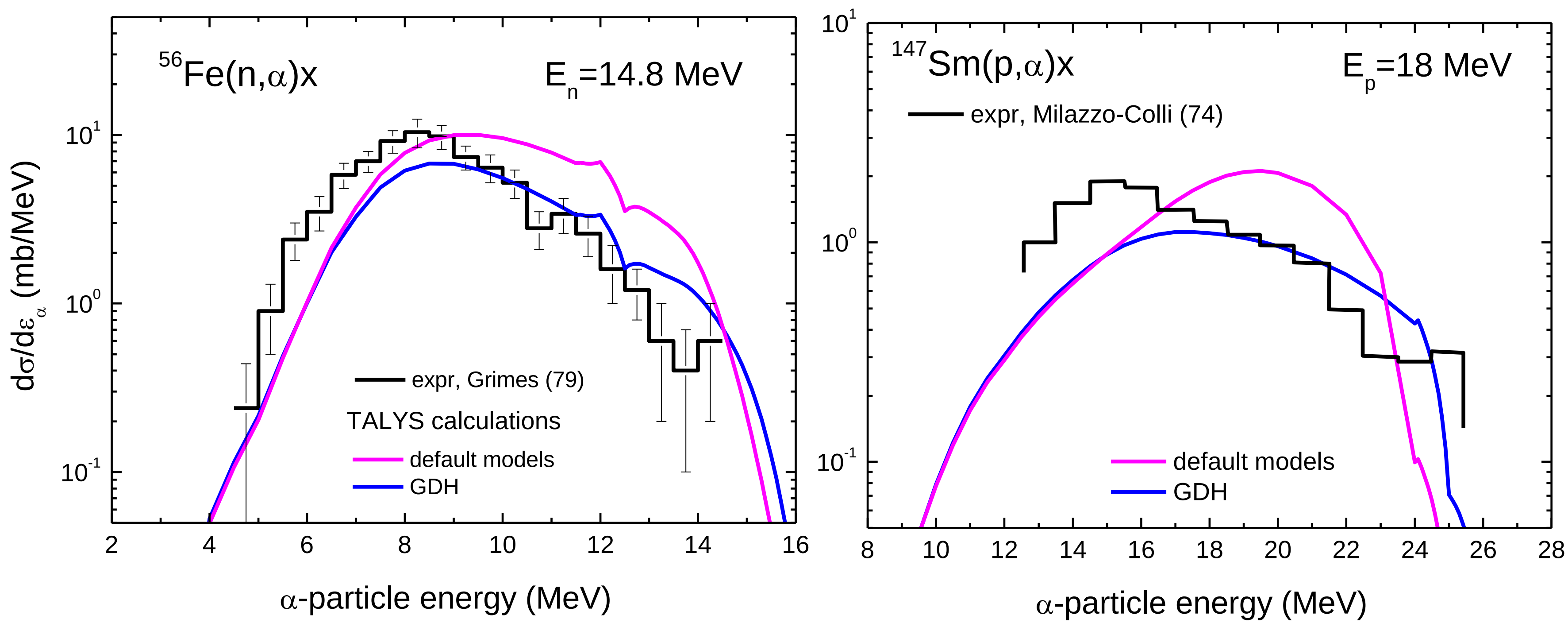


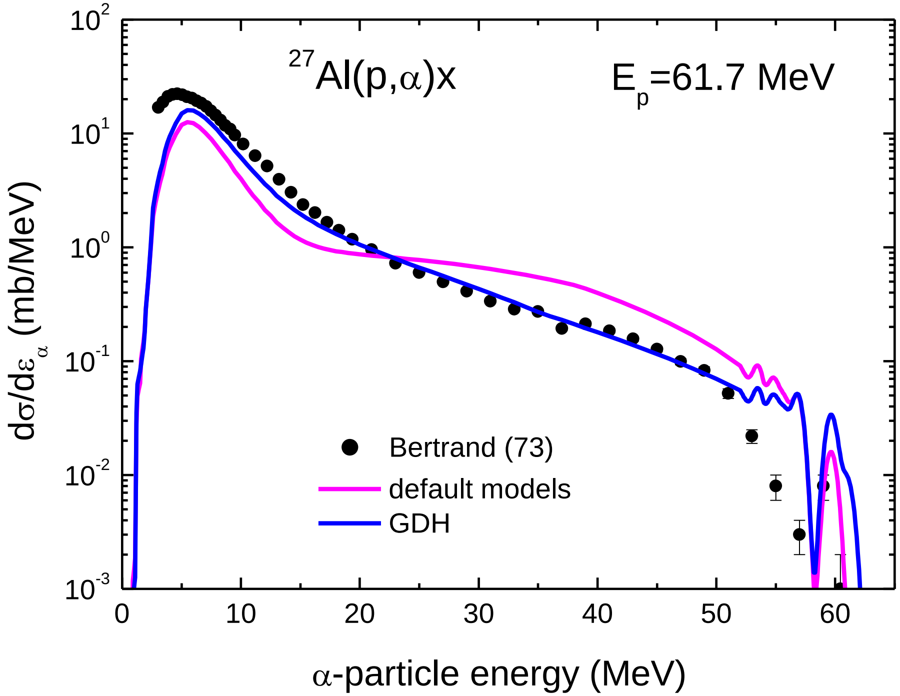




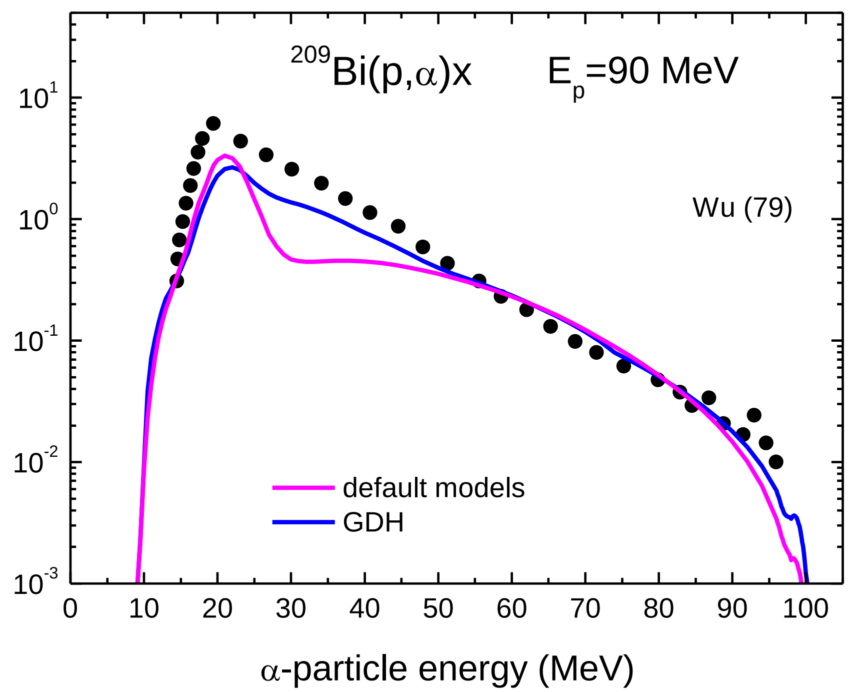
58Ni Ep=90 MeV
Kalend (83)
Wu (79)
(p,p')x
(p,n)x
TALYS calculations
default models
GDH
dσ/dε (mb/MeV)
Nucleon energy (MeV)
90Zr(p,n)x
Ep=160 MeV
Scobel (90)
TALYS calculations
default models
GDH
Neutron energy (MeV)

α-particle energy distributions



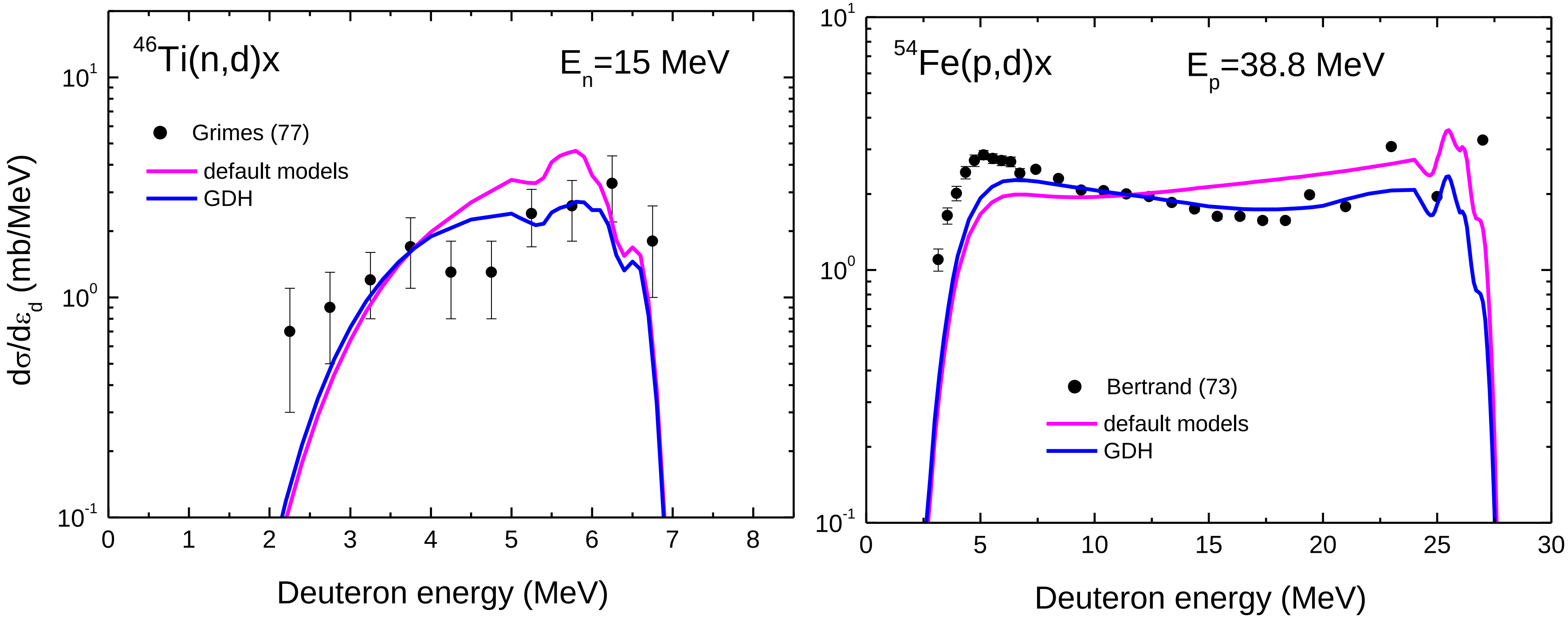


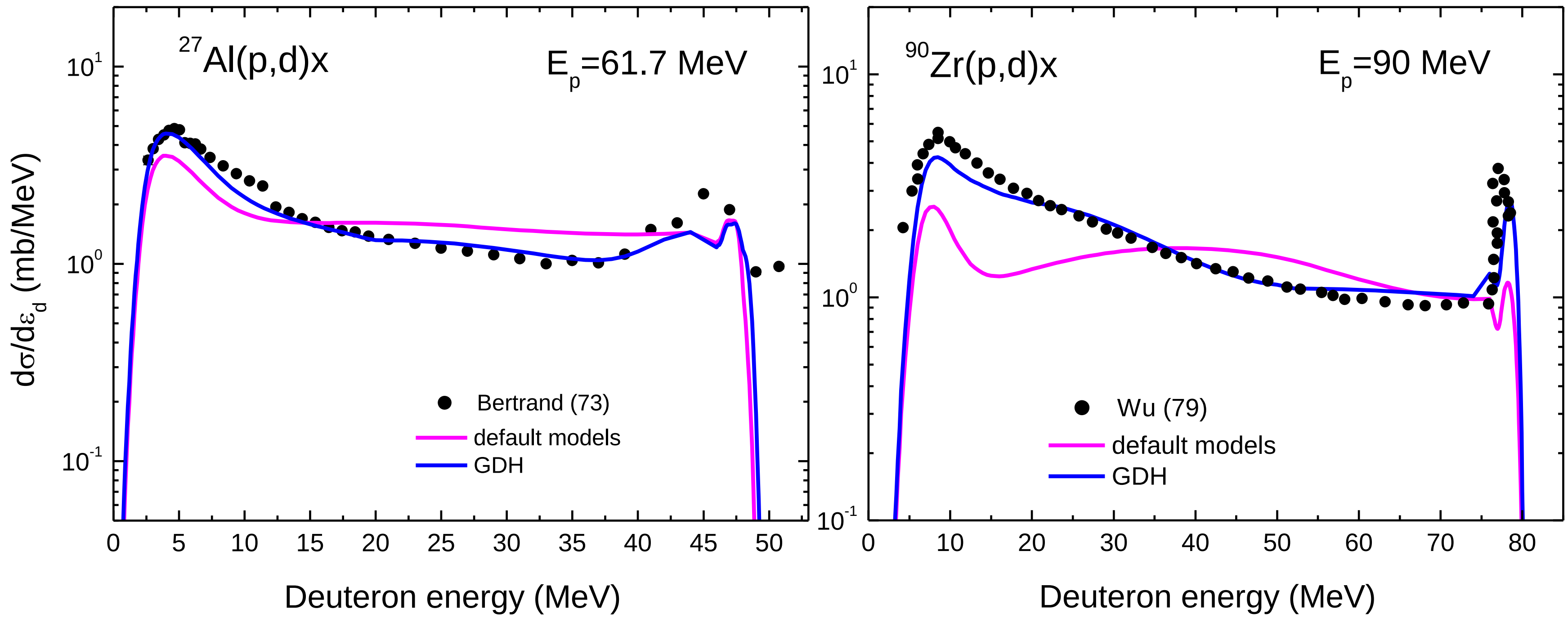
$^{27}Al(p,\alpha)x$
E_p=61.7 MeV
$d\sigma/d\varepsilon_\alpha$ (mb/MeV)
α-particle energy (MeV)
Bertrand (73)
default models
GDH



$^{209}Bi(p,\alpha)x$
E_p=90 MeV
Wu (79)
default models
GDH
α-particle energy (MeV)

Deuteron energy distributions





27Al(p,d)x
Ep=61.7 MeV
dσ/dεd (mb/MeV)
Bertrand (73)
default models
GDH
Deuteron energy (MeV)
90Zr(p,d)x
Ep=90 MeV
Wu (79)
default models
GDH
Deuteron energy (MeV)

Global comparison: (p,x) reaction cross-sections

deviation factors

$$H = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right)^{0.5}$$

$$S = 10^{\left\{ \left(\sum_{i=1}^{N} \left[\frac{\lg(\sigma_i^{exp}) - \lg(\sigma_i^{calc})}{\left(\Delta\sigma_i^{exp} / \sigma_i^{exp}\right)} \right]^2 \right) \left(\sum_{i=1}^{N} \left[\frac{\sigma_i^{exp}}{\left(\Delta\sigma_i^{exp}\right)} \right]^2 \right)^{-1} \right\}^{1/2}}$$

$$R^{CE} = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{calc}}{\sigma_i^{exp}}$$

$$R^{EC} = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{exp}}{\sigma_i^{calc}}$$

$$L = \left[\frac{\sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}} \right)^2}{\sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2} \right]^{0.5}$$

(p,x) reactions, targets Z=12-83, E_p up to 150 MeV, N = 16,045

Factors	default models	GDH	ALICE/ASH
$H = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right)^{0.5}$	20.3	20.9	26.8
$R^{CE} = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{calc}}{\sigma_i^{exp}}$	1.24	1.27	1.27
$R^{EC} = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{exp}}{\sigma_i^{calc}}$	2.33	1.98	832.
$L = \left[\sum_{i=1}^{N} w_i^2 \left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}} \right)^2 \Big/ \sum_{i=1}^{N} w_i^2 \right]^{0.5}$	0.45	0.51	0.60
$S = 10^{\left\{ \left(\sum_{i=1}^{N} \left[\frac{\lg(\sigma_i^{exp}) - \lg(\sigma_i^{calc})}{(\Delta\sigma_i^{exp} / \sigma_i^{exp})} \right]^2 \right) \left(\sum_{i=1}^{N} \left[\frac{\sigma_i^{exp}}{(\Delta\sigma_i^{exp})} \right]^2 \right)^{-1} \right\}^{1/2}}$	1.33	1.33	2.44

The "competition" between exciton model and hybrid model

The discussion seems to be finished

C.A.Soares Pompeia et al, PRC, 2006; ND2007:

Problems with the EM configuration mixing

The solution: HMS model of M.Blann

Complete version soon in EMPIRE, 2010:

competition with TALYS sharpens in physics, spectrum of applications etc.

Proposal

The implementation of HMS model in TALYS

-"all the best in the best code"

-physics

-energy range of application

-emission of particles with A > 4

Conclusion

The GDH model was implemented in TALYS

Test calculations were performed for nuclear reaction cross-sections, nucleon and charged particle energy distributions

The use the GDH model inside of TALYS shows an advantage over ALICE and ALICE/ASH calculations

The implementation of the HMS model in TALYS seems reasonable