IN_TRITIUM PROCESS Project:
Advanced tools for ITER tritium plant systems modelling & design

inprocess Simulation to Business. Knowledge to Profit.

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OUTLINE: **Advanced tritium transfer modelling tools for ITER/DEMO Plant Systems Aspen HYSYS are developed based on our large experience of Chemical Plants Systems modelling; scientific background and tritium expertise.**

Modelling routines for 5key unitary operations for tritium transfer isotopic processes at Plant systems:

(1) isotopic permeation
(2) cold trapping
(3) absorption/desorption
(4) cryodistilation

FACTS

- **System PREDICTIVE MODELLING** is a historical **top level scientific milestone of tritium technology.**
- Tritium **PREDICTIVE MODELLING** is today **a challenge for final design and licensing of T-systems in ITER**.
- **PREDICTIVE MODELLING** impacts on:
  - (1) flexible operational reliability of Plants systems as support for coming dynamic CODAC;
  - (2) safe management and control of extremely large functional complex systems;
  - (3) economy of expensive and scarce fuel.
- Anticipating the future, tritium self-sufficiency demonstration in tritium breeding systems comes from **PREDICTIVE MODELLING**.
- There exist no qualified nuclear tools for ITER and only QA guidelines for their development and use and R&D efforts.

"ADVANCED PREDICTIVE MODELLING" TOOL = UNITARY OPERATIONS MODELLING BASED ON THERMODYNAMIC PRINCIPLES

1ST PRINCIPLES

→ ISOTOPIC DATABASES BASED ON FIRST PRINCIPLES
→ UNDERLYING THERMODYNAMIC MODELING OF UNITARY PROCESSES
→ PREDICTIVITY BASED ON HUGE NUMERIC VALIDATION OF INDUSTRIAL PLANT PROCESSES.
→ UNITARY PROCESS INTEGRATION IN HYPERCOMPLEX SYTEMS NATURAL and MODULAR

[Aspen HYSYS] aspentech

EXPLICIT

→ TRANSPORT DATABASES TO BE ASSUMED "AD HOC"
→ MASS BALANCE EQUATION DESCRIBING SYSTEM PROCESSES TO BE PROGRAMMED
→ PREDICTIVITY TO BE PROVEN "UNITARY PROCESS BY UNITARY PROCESS " THROUGH SPECIFIC BENCHMARKING.
→ DIRECT (HARD) MODULE CONNECTIVE INTEGRATION OR OBJECT PALETIZING

[MATLAB/SIMULINK®, MATHCAD/VISSIM®, ECOSIMPRO®]

MODELLING CASES FOR TRITIUM PLANT UNITARY OPERATION

THERMOPHYSICAL ISOTOPIC DDBBs 1ST PRINCIPLES

	H2	HD	HT	D2	DT	T2
M [uma]	2.016	3.022	4.025	4.029	5.032	6.036
$T_{L\to G}$ [K]	20.39	22.14	22.92	23.67	24.38	25.04
T_{PT} [mm]	13.96	16.60	17.62	18.73	19.71	20.62
$P_{L\to G}$ [mm]	54.0	92.8	109.5	128.6	145.7	162.0
Tc [K]	33.24	35.91	37.13	38.35	39.42	40.44
Pc [bar]	12, 96	14.84	15.70	16.64	17.72	18.49

$$\varphi(r)=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]$$

Parámetros en: [Tc, Pc,Vc]		$\sigma = 2.43\,(T_c/P_c)^{1/3}$			$\varepsilon/\kappa = 0.77\,T_c$ $T^* = T/(\varepsilon/\kappa) = 1.3T/Tc$	
Substancia	M [g/mol]	σ (A)	ε/κ [K]	T_b [K](@1b)	T_c [K]	P_c [bar]
H_2	2.016	3.325	25.595	20.39	33, 24	12, 96
HD	3.022	3.262	27.651	22.14	35.91	14.84
HT	4.025	3.239	28.590	22.92	37.13	15.70
D_2	4.029	3.210	29.530	23.67	38. 35	16.64
DT	5.032	3.172	30.353	24.38	39.42	17.72
T_2	6.034	3.154	31.139	25.04	40.44	18.49

$\sigma = 2.43\,(T_c/P_c)^{1/3}$

$\varepsilon/k_B = 0.77\,T_C$

$T^* = T/(\varepsilon/k_B)$

$$\Omega^{(i,j)*}(T^*)=\frac{2}{(j-1)!\,T^{*(j+2)}}\int_0^\infty exp\left[\frac{-g^{*2}}{T^*}\right]g^{*(2j+3)}Q^{i*}(g^*)\,dg^*$$

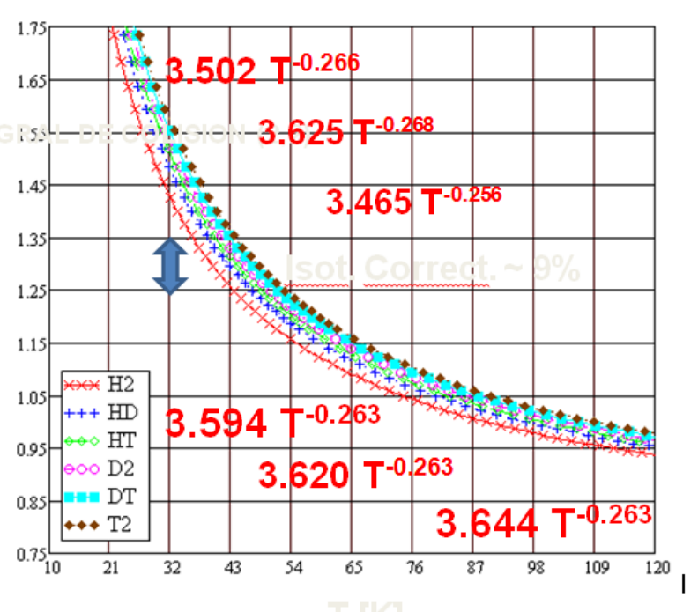
$$Q^{i*}(g^*)=\frac{2}{1-\dfrac{[1-(-1)^i]}{2(1+i)}}\int_0^\infty(1-\cos^i(\chi))\,b^*\,db^*$$

$$\chi(g^*,b^*)=\pi-2b^*\int_0^\infty\frac{dr^*}{r^*\sqrt{1-(b^*)^2(r^*)^{-2}-\varphi^*(r^*)(g^*)^{-2}}}$$

$$\Omega^{(l,s)*}(T^*)=\left(\frac{A}{T^*}\right)+[C\exp(-DT^*)]+[E\exp(-FT^*)]+[G\exp(-HT^*)]+RT^{*B}\sin(ST^{*W}-P)$$

(l,s)	A	B	C	D	E	F	G	H	Rx10⁴	S	W	P
(1,1)	1,06036	0,15610	0.19300	0,47365	1,03587	1,52996	1,76747	3,89411	--------	-----	----	----
(2,2)	1,16145	0,14874	0.52487	0,77320	2,16178	2,43787	---------	---------	-6.435	18.032	-0.768	7.2773

T* [-]	$\Omega^{(1,1)}$	$\Omega^{(2,2)}$
2.8	0.9681	1.0591
2.9	0.9588	1.0489
3.0	0.9500	1.0394
3.1	0.9418	1.0304
3.2	0.9341	1.0220
3.3	0.9268	1.0141
3.4	0.9199	1.0066
3.5	0.9133	0.9995
3.6	0.9071	0.9927
3.7	0.9012	0.9864
3.8	0.8956	0.9803
3.9	0.8902	0.9745
4.0	0.8850	0.9690
4.1	0.8801	0.9637
4.2	0.8753	0.9587
4.3	0.8708	0.9539
4.4	0.8664	0.9493
4.5	0.8622	0.9448
4.6	0.8581	0.9406
4.7	0.8541	0.9365
4.8	0.8503	0.9326
4.9	0.8467	0.9288
5.0	0.8431	0.9252
6.0	0.8128	0.8948
7.0	0.7895	0.8719
8.0	0.7707	0.8535
9.0	0.7551	0.8382
10.0	0.7419	0.8249
12.0	0.7201	0.8026
14.0	0.7026	0.7844
16.0	0.6879	0.7690
18.0	0.6753	0.7556
20.0	0.6643	0.7439
25.0	0.6416	0.7196
30.0	0.6236	0.7003
35.0	0.6087	0.6844
40.0	0.5962	0.6710
50.0	0.5758	0.6491
75.0	0.5405	0.6111
100.0	0.5167	0.5855
150.0	0.4850	0.5512



$$\mu=2.6693\cdot10^{-6}\frac{\sqrt{MT}}{\sigma^2\Omega^{(2,2)}}$$

$$\lambda=8.3254\cdot10^{-2}\frac{\sqrt{\frac{T}{M}}}{\sigma^2\Omega^{(2,2)}}$$

$$D(T)=\frac{26.28\cdot10^{-2}}{p}\frac{\sqrt{\frac{T^3}{M}}}{\sigma^2\Omega^{(1,1)}}$$

	H2	HD	HT	D2	DT	T2
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T (K)	D(H_2,He)	D(HD,He)	D(D_2,He)	D(HT,He)	D(DT,He)	D(T_2,He)
298,1	$7.0\ 10^{-4}$	$6.1\ 10^{-4}$	$5.7\ 10^{-4}$	$5.1\ 10^{-4}$	$4.3\ 10^{-4}$	$3.6\ 10^{-4}$
300	$8.2\ 10^{-4}$	$7.2\ 10^{-4}$	$6.8\ 10^{-4}$	$6.5\ 10^{-4}$	$5.8\ 10^{-4}$	$4.7\ 10^{-4}$
400	$1.0\ 10^{-3}$	$9.2\ 10^{-4}$	$8.8\ 10^{-4}$	$8.4\ 10^{-4}$	$7.1\ 10^{-4}$	$6.1\ 10^{-4}$
500	$2.2\ 10^{-3}$	$1.1\ 10^{-3}$	$9.9\ 10^{-4}$	$9.2\ 10^{-4}$	$8.2\ 10^{-4}$	$7.7\ 10^{-4}$
600	$3.2\ 10^{-3}$	$2.3\ 10^{-3}$	$2.1\ 10^{-3}$	$1.8\ 10^{-3}$	$1.1\ 10^{-3}$	$9.8\ 10^{-4}$

	H_2O	HDO	D_2O	T_2O	HTO
T [ºC]	100.00	101.28	101.42	101.51	101.8
Pres. Vap (mm Hg) @25 ºC	23.76	22.12	20.6	19.8	17.2
Temperatura [ºC]	H_2O	HDO	D_2O	T_2O	HTO
25	1	1.075	1.154	1.193	1.095
50	1	1.053	1.110	1.134	1.065
100	1	1.026	1.052	1.064	1.030

	300ºC	350 ºC	400ºC	450ºC	500ºC
H2+T2←→2HT	4.83		5.27		5.49
HT+H2O←→H2 + HTO	2.058	1.879	1.741	1,632	1.545
T2+H2O←→ HT+HTO	10.09		9.16		8.34

Van Hook; Journal of Chemistry Physics 72, 1234 (1968)

a[A]+b[B] ←→ c[C]+d[D]

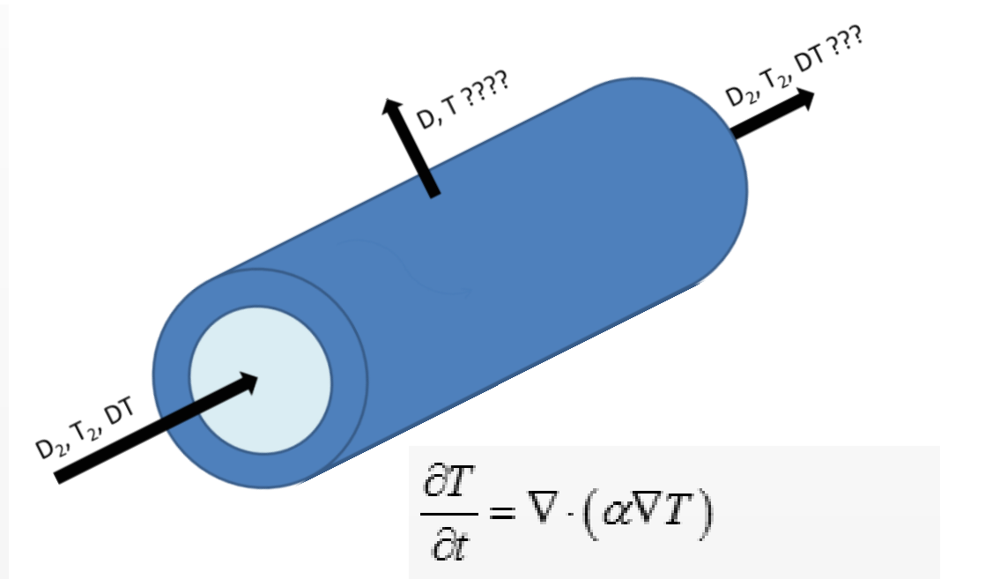
$$R=K_f\left([A]^a[B]^b-\frac{1}{K_{eq}}[C]^c[D]^d\right)$$

- $K_1(T_2, H_2O \leftrightarrow HTO, HT) = 2.e^{-29}([T_2][H_2O] - [HTO][HT]/Keq(1))$
- $K_2(HT, H2O \leftrightarrow HTO, H_2) = 1.e{-29}([HT]\,[H2O] - [HTO]\,[H2]\,/Keq(2))$

ISOTOPIC MULTI-SPECIES NOMINAL PERMEATION WITH HYSYS

aspentech

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(v\rho)=0$$
$$\frac{\partial\rho v}{\partial t}+(\rho v\cdot\nabla)v=-\nabla p+\nabla\cdot(\mu\nabla v)+\rho g$$
$$\frac{\partial\rho h}{\partial t}+(\rho v\cdot\nabla)h=-\frac{Dp}{Dt}+\nabla\cdot\left(\frac{k}{c_p}\nabla h\right)$$
$$\frac{\partial C_{Y_2}}{\partial t}+\nabla\cdot(vC_{Y_2})=\nabla\cdot(D_{Y_2}\nabla C_{Y_2})+S_{Y_2}$$
$$\frac{\partial C_{XY}}{\partial t}+\nabla\cdot(vC_{XY})=\nabla\cdot(D_{XY}\nabla C_{XY})+S_{XY}$$
$$\frac{\partial C_{X_2}}{\partial t}+\nabla\cdot(vC_{X_2})=\nabla\cdot(D_{X_2}\nabla C_{X_2})+S_{X_2}$$



$$\frac{\partial T}{\partial t}=\nabla\cdot(\alpha\nabla T)$$
$$\frac{\partial C_X}{\partial t}=\nabla\cdot(D_X\nabla C_X)+S_X$$
$$\frac{\partial C_Y}{\partial t}=\nabla\cdot(D_Y\nabla C_Y)+S_Y$$

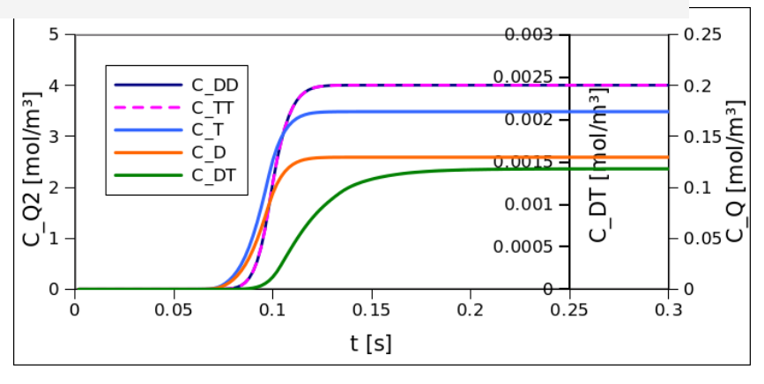
Fluid → solid

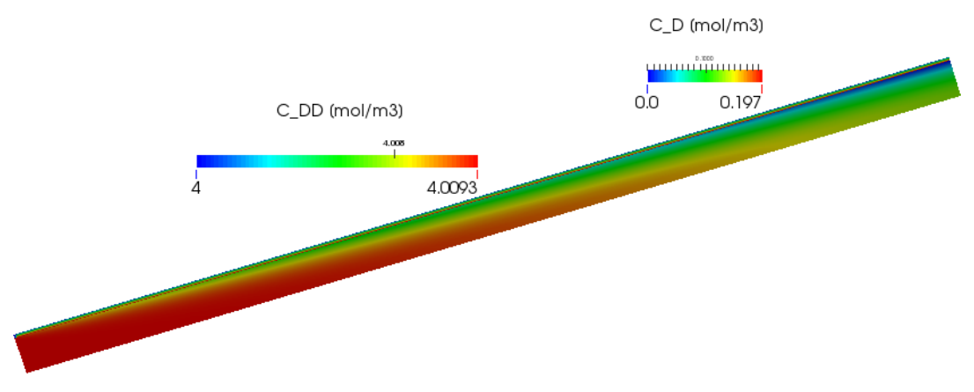
$$-D_{X_2}\nabla C_{X_2}=J_{X_2}=k_{d,X_2}P_{X_2}-k_{r,X_2}(C_X)^2$$
$$-D_{XY}\nabla C_{XY}=J_{XY}=k_{d,XY}P_{XY}-k_{r,XY}C_XC_Y$$
$$-D_{Y_2}\nabla C_{Y_2}=J_{Y_2}=k_{d,Y_2}P_{Y_2}-k_{r,Y_2}(C_Y)^2$$
$$-D_X\nabla C_X=J_X=2J_{X_2}+J_{XY}$$
$$-D_Y\nabla C_Y=J_Y=2J_{Y_2}+J_{XY}$$

Solid → atmosphere

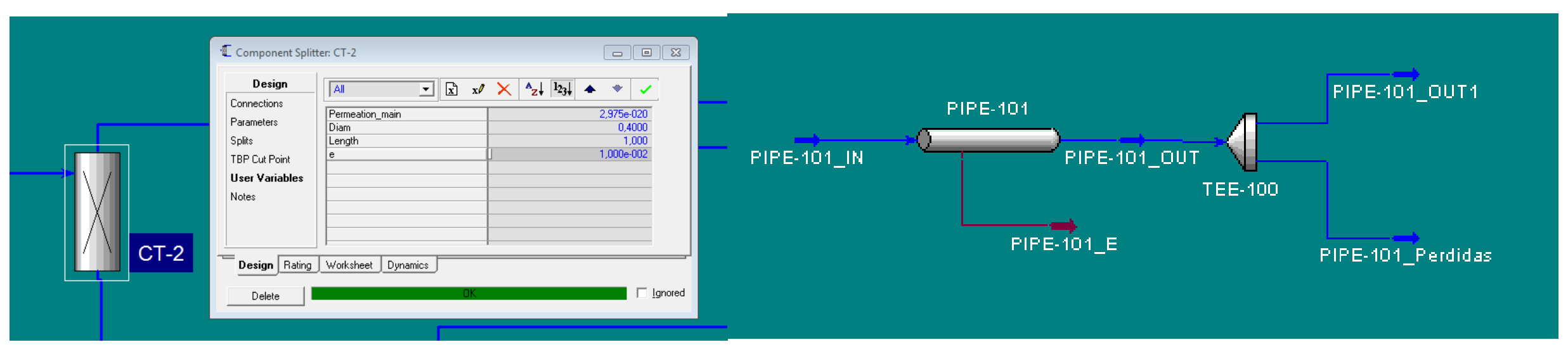
$$J_{X_2,ext}=k_{r,X_2,ext}(C_X)^2$$
$$J_{XY,ext}=k_{r,XY,ext}C_XC_Y$$
$$J_{Y_2,ext}=k_{r,Y_2,ext}(C_Y)^2$$
$$-D_X\nabla C_X=J_{X,ext}=2J_{X_2,ext}+J_{XY,ext}$$
$$-D_Y\nabla C_Y=J_{Y,ext}=2J_{Y_2,ext}+J_{XY,ext}$$

D (Q_2)	6,6e-4	m^2/s
D (T)	2,0e-8	m^2/s
D (D)	2.45e-8	m^2/s
ks (Q)	3.5e-3	$mol/(m^3\cdot Pa^{0,5})$
kd (T_2)	3,18e-8	$mol\cdot s/(m\cdot kg)$
kd (DT)	3,49e-8	$mol\cdot s/(m\cdot kg)$
kd (D_2)	3,90e-8	$mol\cdot s/(m\cdot kg)$
kr (T_2)	2,6e-3	m^4/s
kr (DT)	5,78e-3	m^4/s
kr (D_2)	3,18e-3	m^4/s





case 2	$J_{D2,in}$	$J_{D2,w}$	$J_{DT,in}$	$J_{DT,w}$	$J_{T2,in}$	$J_{T2,w}$	S_{D2}	S_{DT}	C_{D2}
	[mol/s]						[mol]		[mol/m³]
1	7.06e-5	3.18e-9	--	--	--	--	8.74e-5	--	4.0093
2	7.06e-7	3.12e-9	1.8e-13	-5.9e-9	7.06e-7	3.15e-9	8.74e-7	6.2e-10	0.0401
3	7.06e-5	3.06e-7	3.1e-11	-6.1e-7	7.06e-5	3.06e-7	8.74e-5	6.33e-8	4.0078
4	7.06e-5	5.87e-9	1.41e-4	-6.5e-9	7.06e-5	5.93e-9	8.74e-5	1.75e-4	4.0093



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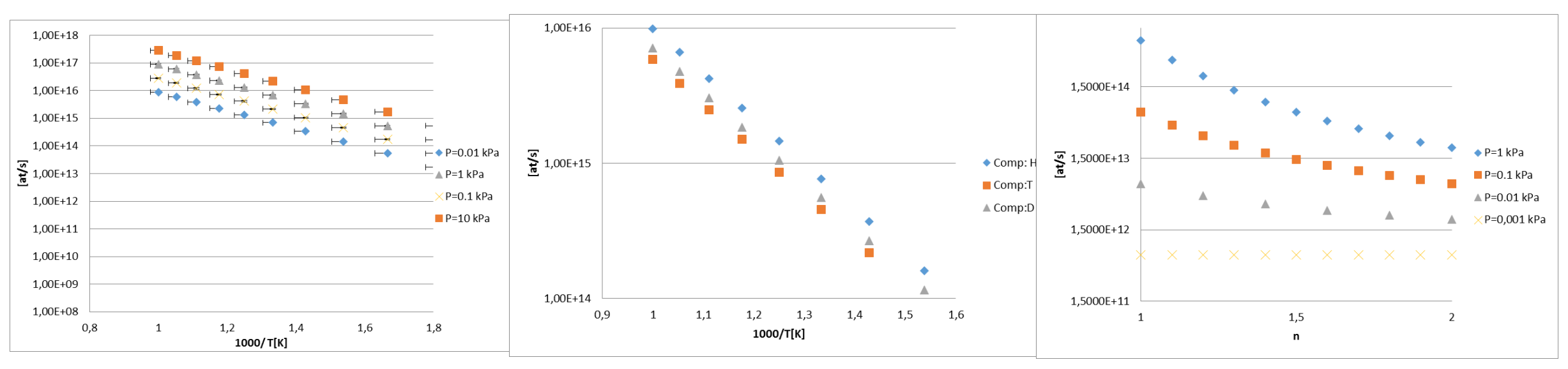
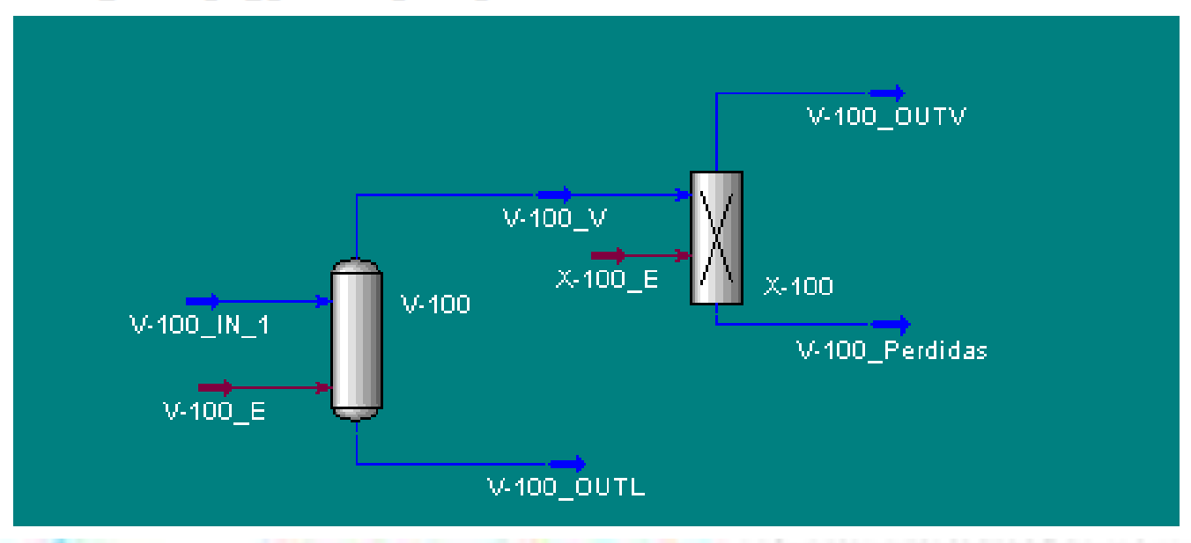
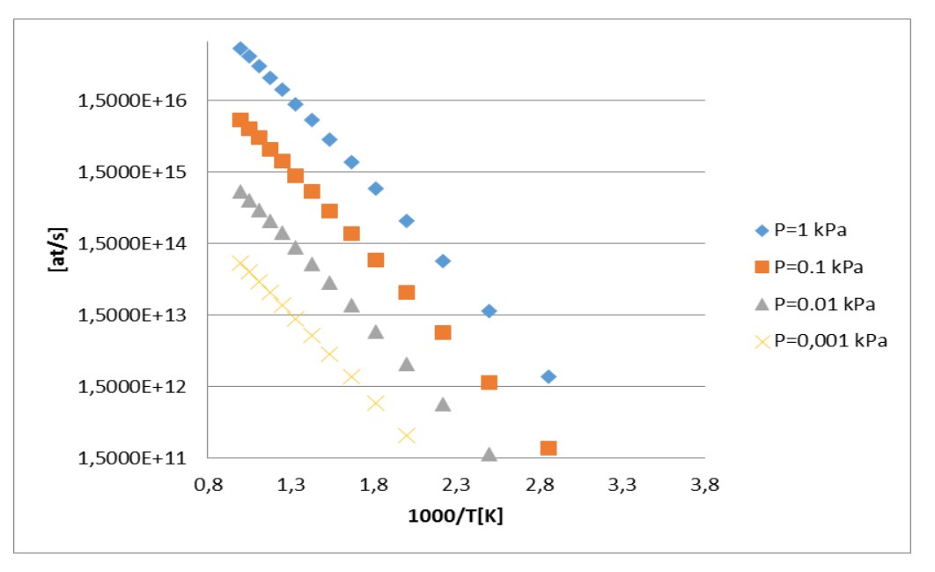


CO-STREAM ISOTOPIC SWAMPING FROM EQUILIBRIUM

$$[H_2]+[T_2]\overset{eq}{\leftrightarrow}2[HT]$$





ABSORPTION//DESORPTION MODELLING WITH HYSYS

REGENERATIVE COLD TRAPPING MODELLING

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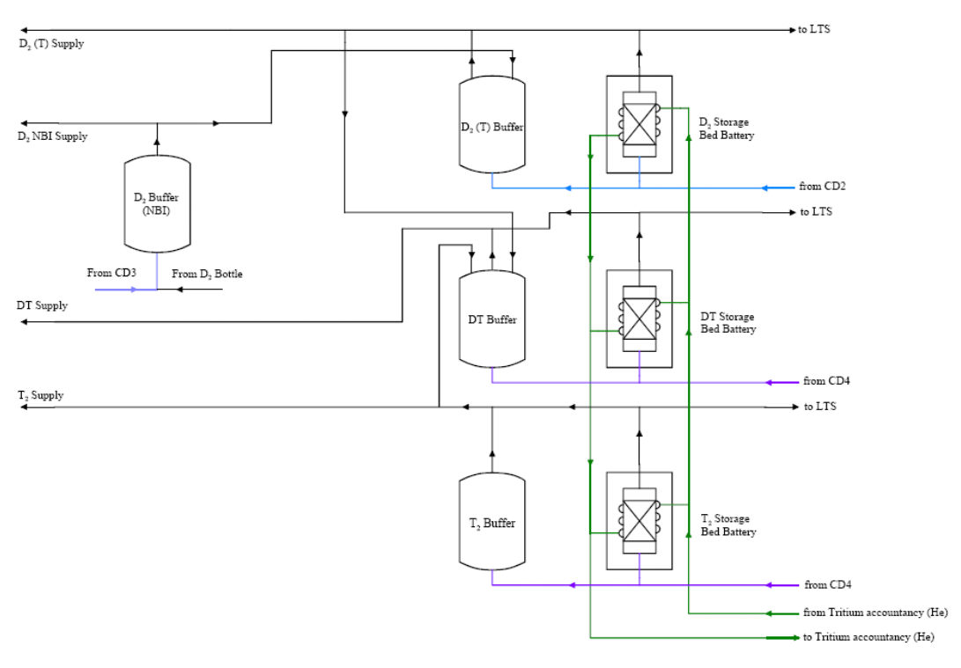
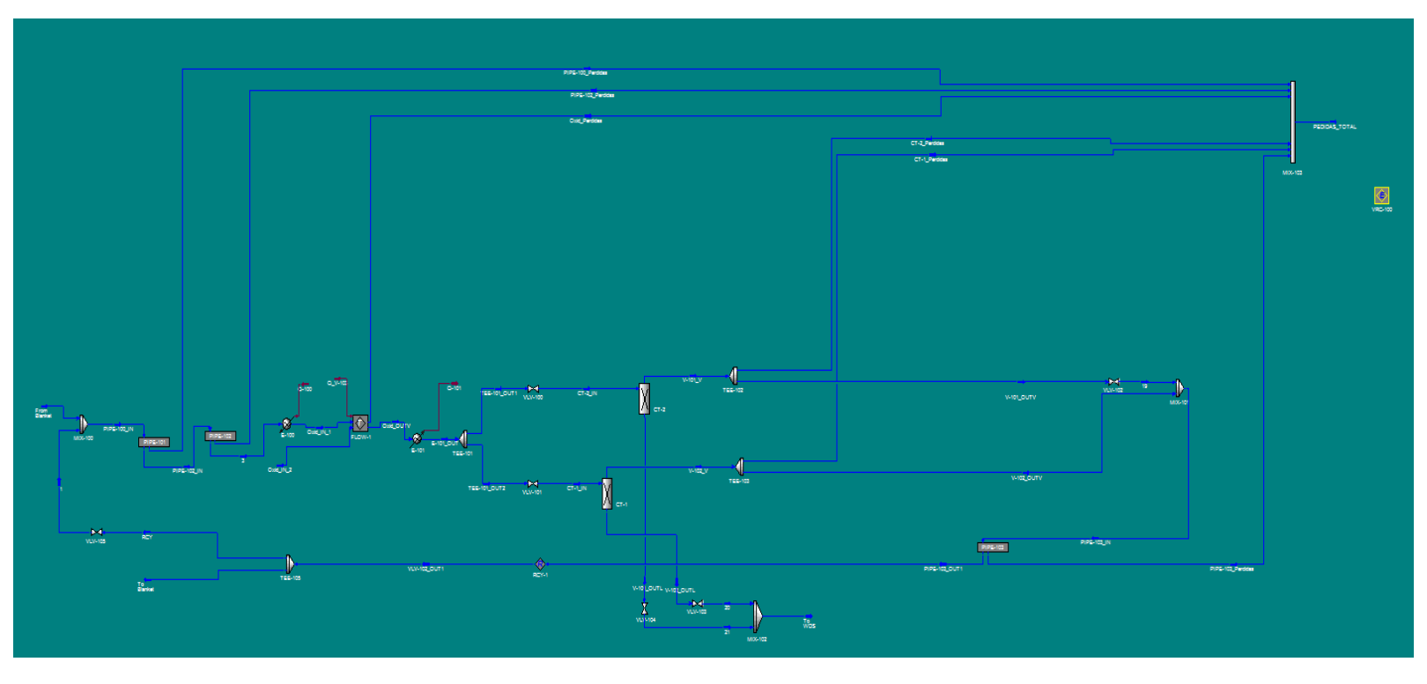
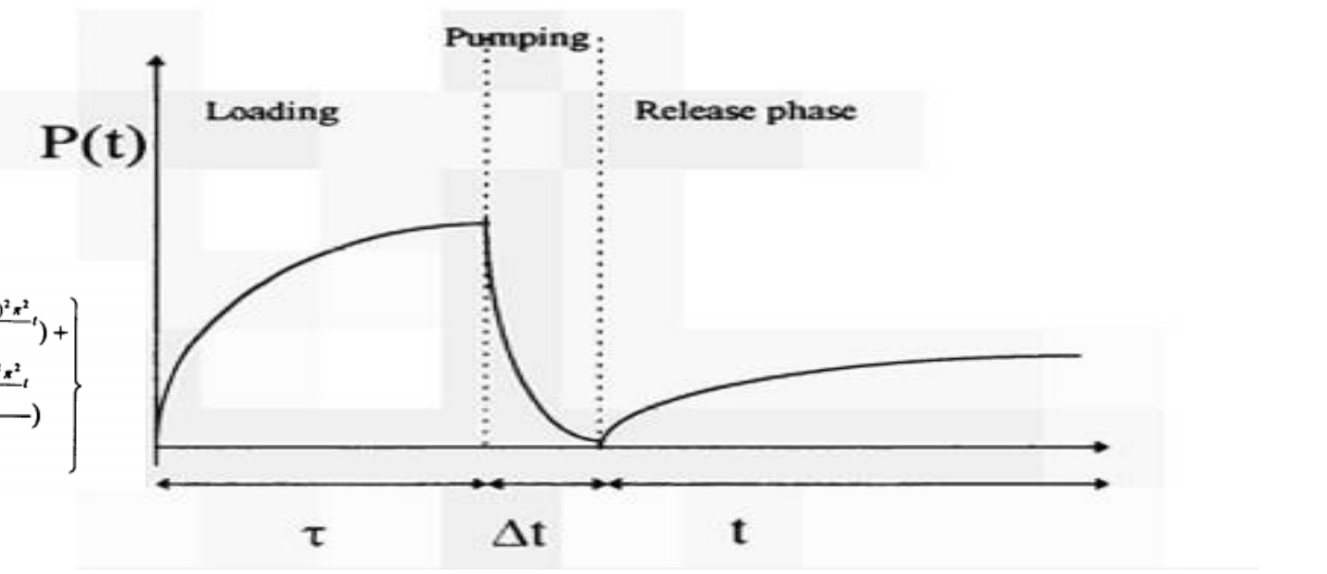


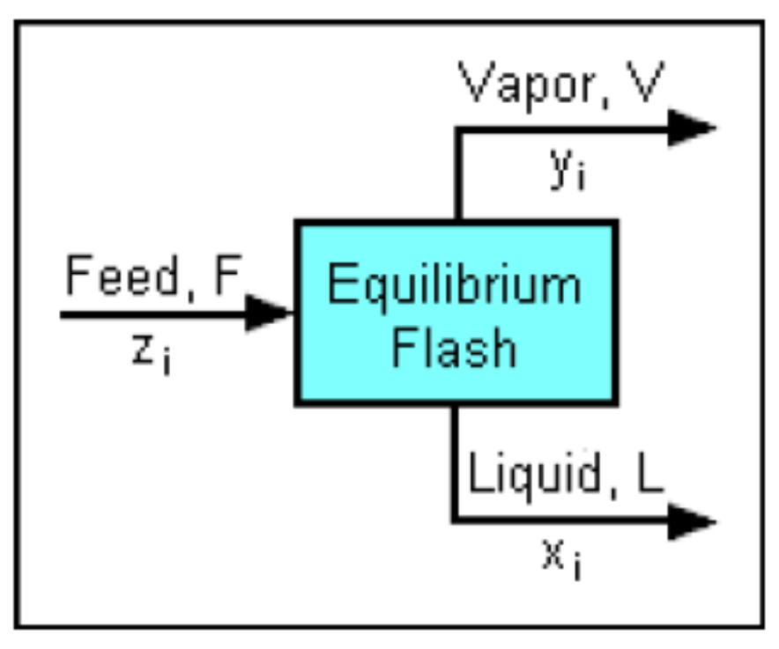


- $U + 3T_2 \rightarrow UT_6 + Q\uparrow$
- $UT_6 + Q \rightarrow U + 3T_2$

$$p(t)=\frac{RT}{(V_1-4V_S).2.N_A}.V_s\frac{8}{\pi^2}\sum_{m=0}^{\infty}\frac{1}{(2m+1)^2}\left\{\begin{array}{l}\Psi_n(\tau,\Delta t)(1-e^{-\frac{D(2m+1)^2\pi^2}{l^2}t})+c_{\Delta t}(1-e^{-\frac{D(2m+1)^2\pi^2}{l^2}t})+\\+\frac{c_f-c_{\Delta t}}{1-e^{-\gamma\tau}}(1-e^{-\frac{D(2m+1)^2\pi^2}{l^2}t}-\frac{e^{-\gamma t}-e^{-\frac{D(2m+1)^2\pi^2}{l^2}t}}{1-\gamma/D\alpha_n^2})\end{array}\right\}$$



MODELLING FLASH (HYSYS)

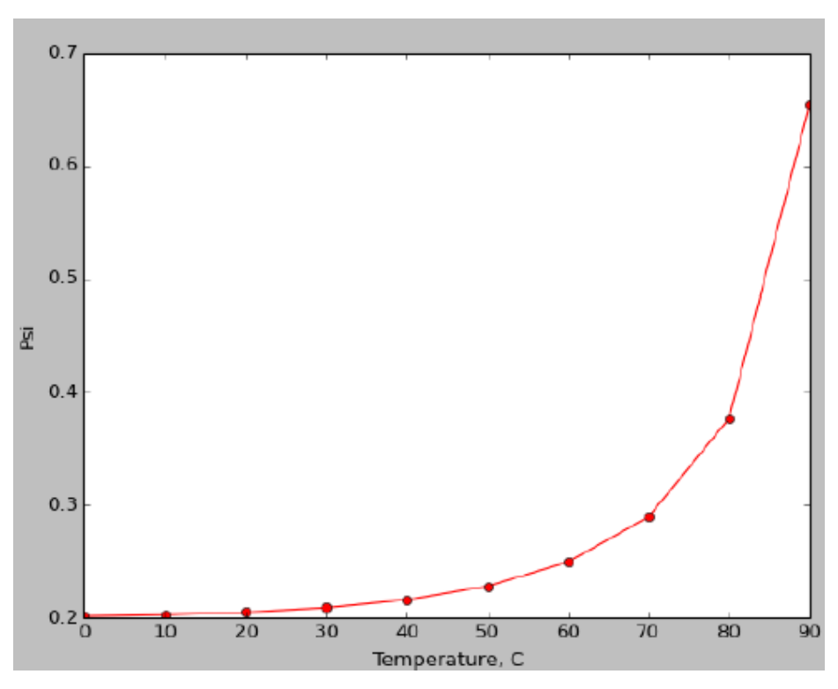


$K_i = y_i/x_i$

$L+V=1$

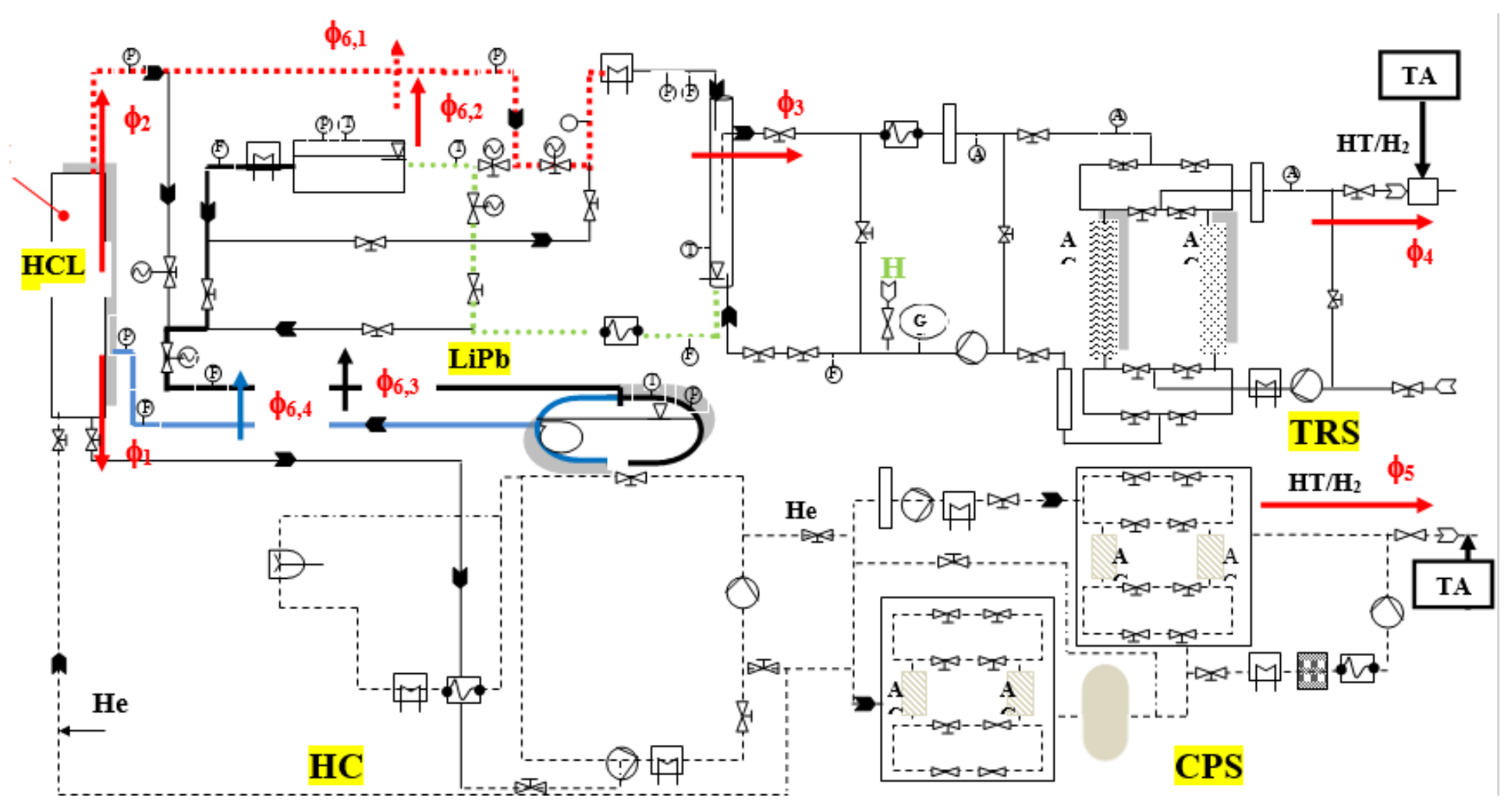
$z_i = x_iL + y_iV$

$$y_i=\frac{z_iK_i}{1+V(K_i-1)}$$



[HTO (v) saturating H_2O]

TOWARDS ULTRACOMPLEXE SYSTEMS



ONGOING CONCLUSIONS

→ **TRITIUM PLANT UNITARY OPERATIONS MODELLED ON THE BASIS OF FIRST THERMODYNAMIC PRINCIPLES**

→ **IMPLEMENTED IN ASPEN/HYSYS ROUTINES**

→ **INTEGRATION INTO FULL PLANT SYSTEM COMPLEXITY ONGOING.**

POSTER **ID 5-17**

MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

CDTI Centro para el Desarrollo Tecnológico Industrial

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