Status of the ISTC project #3345 “Ex-vessel source term analysis” (EVAN)”, phase 1

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Project work packages

- **WP1: Analysis of Severe Accident Scenarios (SPAEP, IBRAE)**

- **WP2: FP release from molten corium pool**
  - **Task 2: Experimental investigations (NITI)**
  - **Task 3: Theoretical and numerical modeling (IBRAE)**

- **WP 3: Primary aerosol transport/deposition**
  - **Task 4: Experimental investigations (NPO CKTI)**
  - **Task 5: Theoretical and numerical modeling (SPAEP, IBRAE)**

- **WP 4: Containment parameters impact on iodine species behaviour**
  - **Task 6: Experimental investigations (VNIPIET)**
  - **Task 7: Theoretical and numerical modeling (VNIPIET, SPAEP)**

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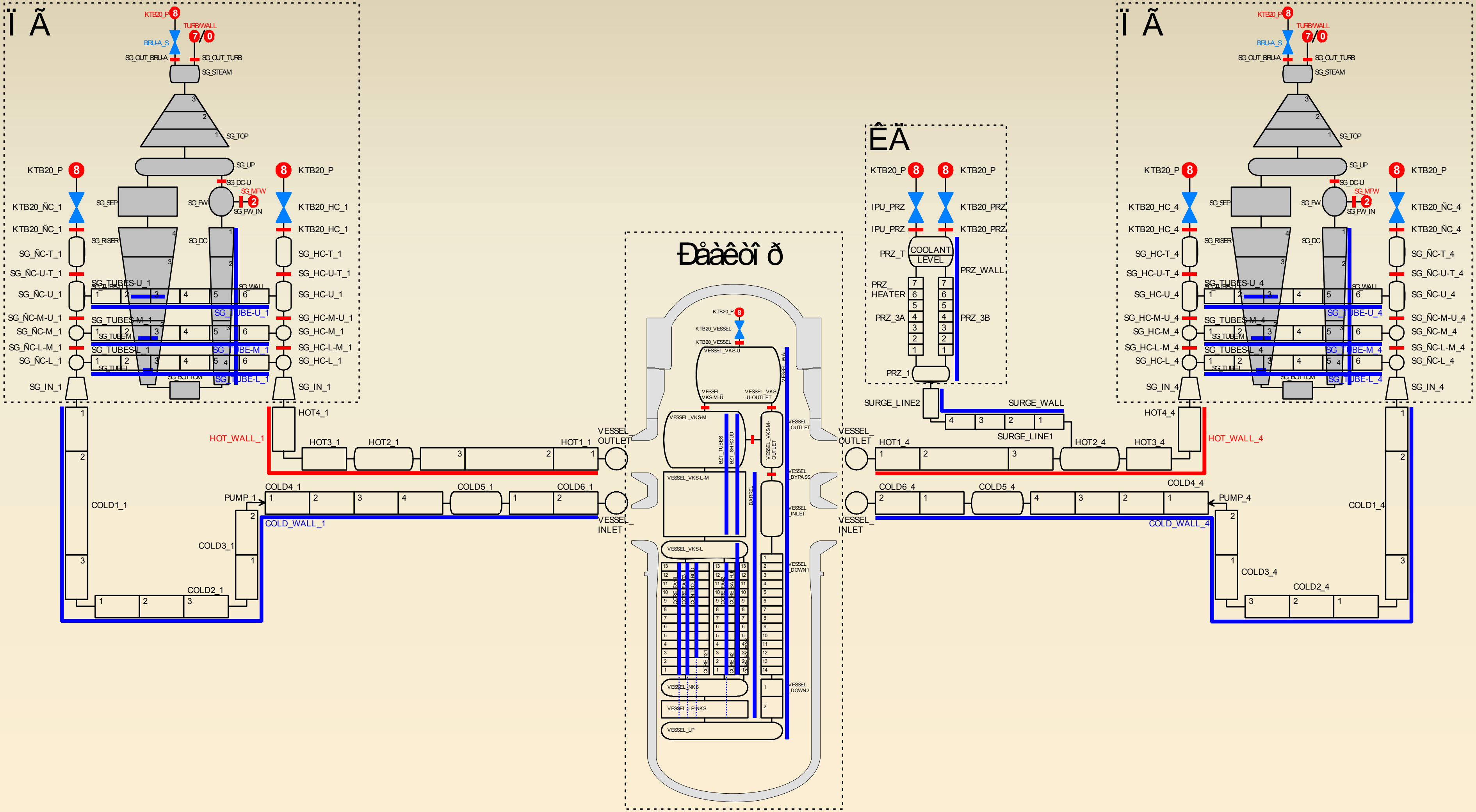
WP1:Fission products inventories (VVER, PWR)

Fission products	Mass, %	Activity at 0 days, %	Activity at 30 days, %
Xe	0,44	3,9	0,4
I	0,02	5,2	0,7
Cs	0,2	3,5	1,3
Ru	0,19	1,7	9,7
Sr	0,07	4,2	6,7
Mo	0,27	3,9	0,01
Ba	0,14	4,4	2,9
Ce	0,23	3,3	15,3
La	0,1	4,8	0,0
summ	1,7	35	37

After 3 years of operation, Birnup: 45 GW/t of UO_2

WP1:Nodalization scheme of WWER-1000 NPP



WP1:Phases of in –vessel stage of severe accident (Large LOCA:D=346 mm)

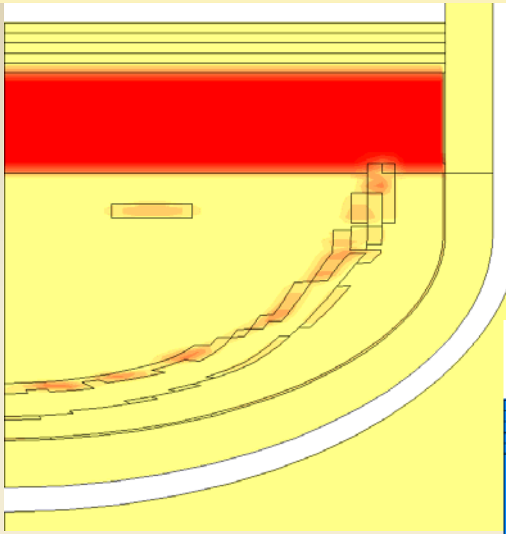
Key stages of accident propagation	Time, s
Commencement of core dry-out	12
Actuation of ECCS accumulators in case of pressure drop in RPV down to 5.9 MPa (supply of borated solution in the upper and lower chambers of the reactor)	55
Re-filling of the core	80
Disconnection of ECCS accumulators	137
Commencement of re-dry-out of the core	140
Commencement of core heat-up	910
Commencement of hydrogen generation	1000
FA cladding temperature is in excess of the design threshold (1473 К)	1607
Complete re-dryout of the core	1560
Degradation of film ZrO2 of FA claddings (Т>2250К)	2328
Release of the materials of the damaged part of the core and internals into the reactor lower chamber	2015
Generation of local melt baths in the core. Excess of fuel melting temperature in the degraded part of the core (T>2850K)	2570
Melt-through of the suspended reactor shaft barrel at the reactor bottom	6170
RPV failure. Release of the first portion of corium into the core catcher.	8345

WP1: Phases of in-vessel stage of accident (Small LOCA: D=25 mm)

Key stages of accident propagation	Time, s
Commencement of core dry-out	1200
Actuation of ECCS accumulators in case of pressure drop in RPV down to 5.9 MPa (supply of borated solution in the upper and lower chambers of the reactor)	7700
Re-filling of the core	7700
Commencement of core heating	12500
Disconnection of ECCS accumulators	13800
Commencement of re-dryout of the core	13900
Commencement of intensive hydrogen generation	15200
Temperature of FA cladding is in excess of design limit (1473 К)	15650
Degradation of film ZrO2 of FA cladding (Т>2250К)	16160
Complete re-dryout of the core	16400
Commencement of release of materials of degraded part of the core and internals into the lower plenum chamber	17445
Formation of local corium baths in the core. Excess of fuel melting temperature in the damaged part of the core (T>2850K)	19300
Melt-through of the suspended reactor shaft barrel. Release of corium onto the reactor bottom	26788
RPV failure, release of the first portion of corium into the core catcher.	29810

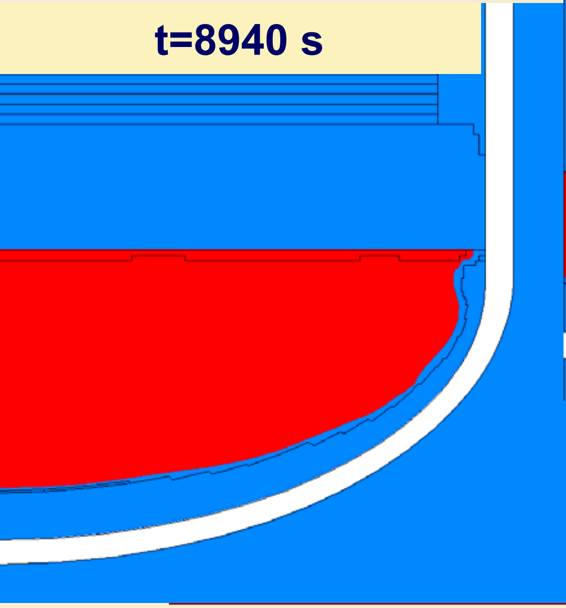
WP1: Melt structure at the reactor bottom during large LOCA

Distribution of steel, t=6200 s

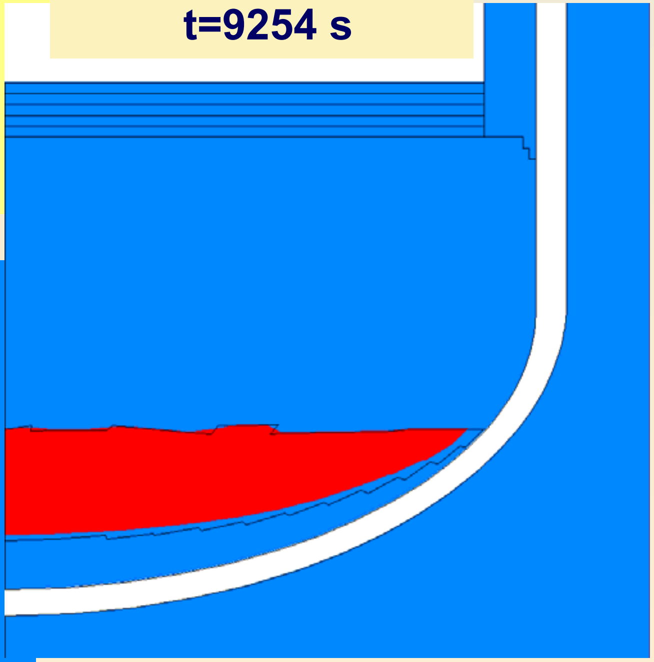


Molten pool evolution during melt release

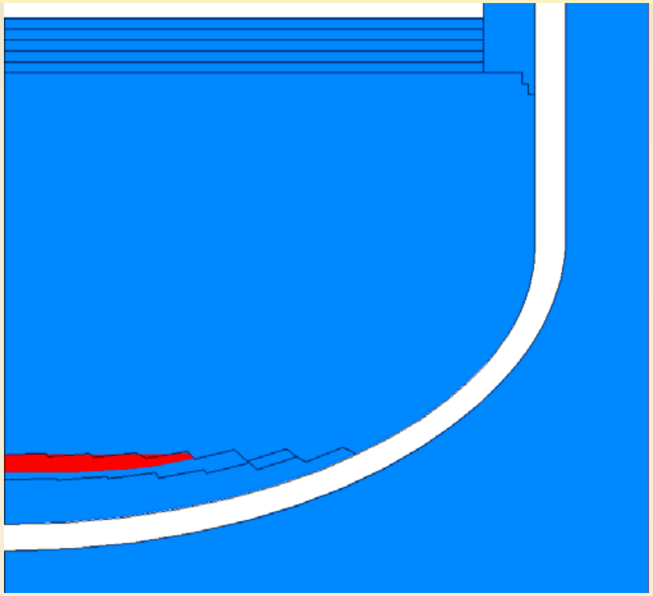
t=8940 s



t=9254 s



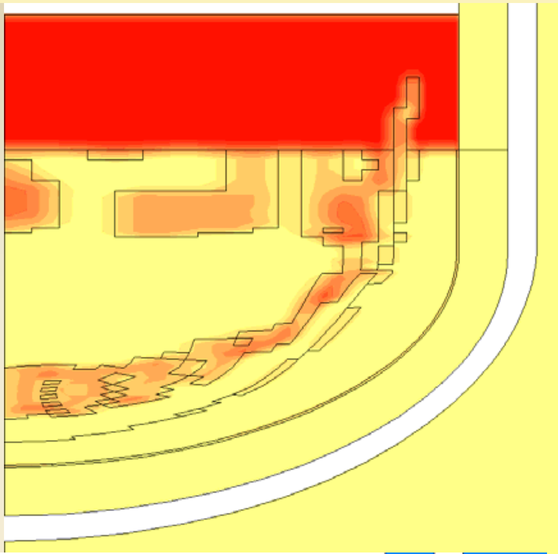
t=11190 s



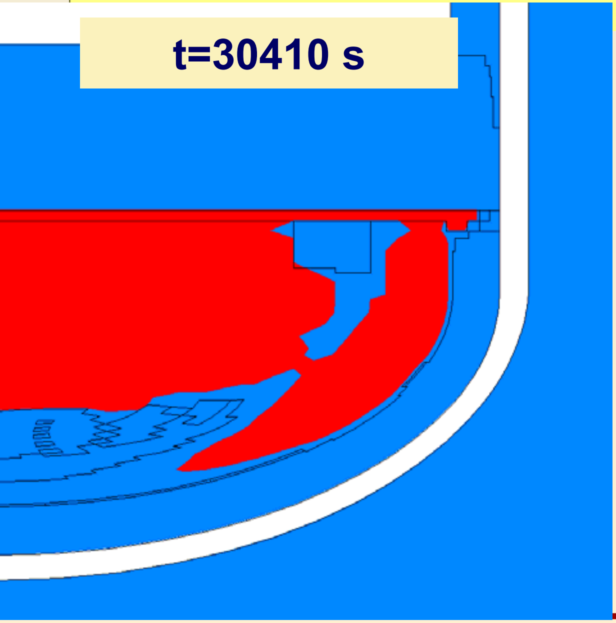
WP1: Parameters of melt during large LOCA

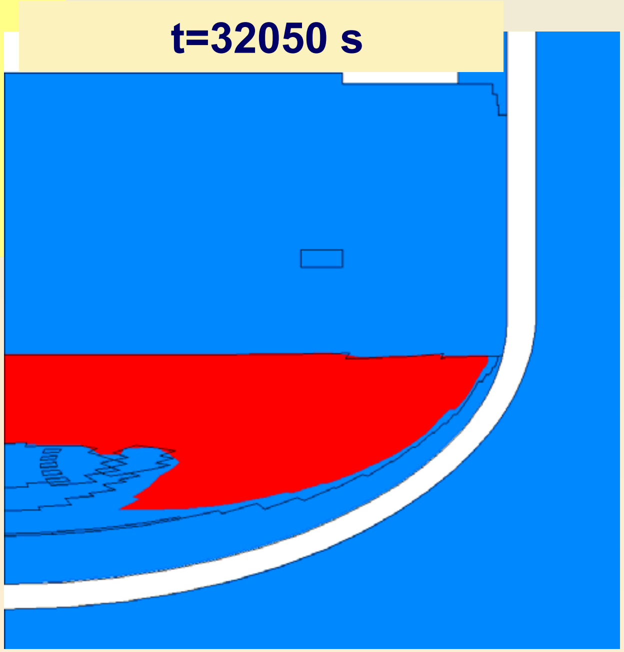
Time, s	Structure of melt, mass fraction	Temperature, К
6 200	Metallic layer: Steel = 0,928; Zr = 0,072 Oxidic layer: UO2 = 0,786; ZrO2 = 0,118; Zr = 0,096	3010-2900 2900-2850
8 955	UO2 = 0,720; ZrO2 = 0,108; Zr = 0,052; Steel = 0,120	3060-2780
9 155	UO2 = 0,682; ZrO2 = 0,102; Zr = 0,049; Steel = 0,167	3050-2780
9 370	UO2 = 0,650; ZrO2 = 0,097; Zr = 0,047; Steel = 0,206	3020-2700
10 224	UO2 = 0,533; ZrO2 = 0,080; Zr = 0,038; Steel = 0,349	2900-2600
11 820	End of melt relocation	

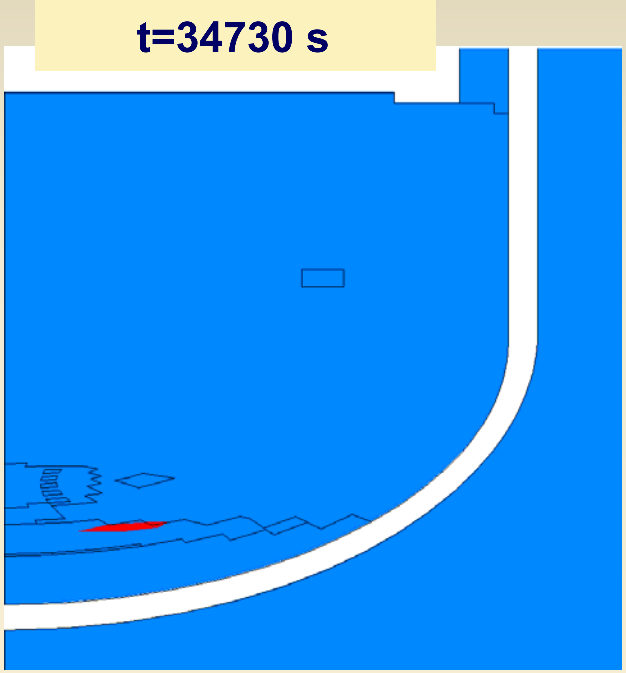
WP1: Melt structure at the reactor bottom during small LOCA


Distribution of steel, t=26 800 s

Molten pool evolution during melt release


t=30410 s


t=32050 s


t=34730 s

WP1: Parameters of melt during small LOCA

Time, s	Structure of melt, mass fraction	Temperature, K
26 800	Metallic layer : Steel = 0,94; Zr = 0,06 Oxidic layer : UO2 = 0,779; ZrO2 = 0,208; Zr = 0,13	2940-2880 2880-2750
31 560	UO2 = 0,627; ZrO2 = 0,199; Zr = 0,007; Steel = 0,167	2900-2750
32 060	UO2 = 0,577; ZrO2 = 0,183; Zr = 0,006; Steel = 0,234	2880-2700
32 540	UO2 = 0,542; ZrO2 = 0,166; Zr = 0,003; Steel = 0,289	2880-2630
32 940	UO2 = 0,503; ZrO2 = 0,154; Zr = 0,003; Steel = 0,341	2720-2620
34 400	UO2 = 0,434; ZrO2 = 0,133; Zr = 0,002; Steel = 0,431	2540
36 000	End of melt relocation	

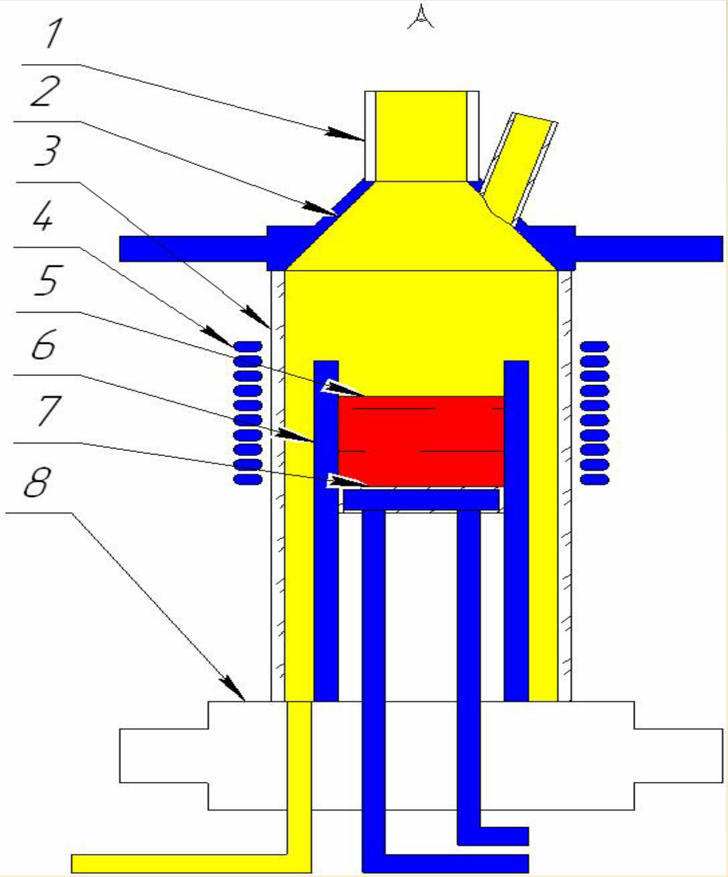
WP2: Experiment EVAN-FP1

Test objective

Determination of release rates of fission product simulants and melt components at corium oxidation transient from C70 to C100

WP2: Experiment EVAN-FP1

Furnace for melt generation

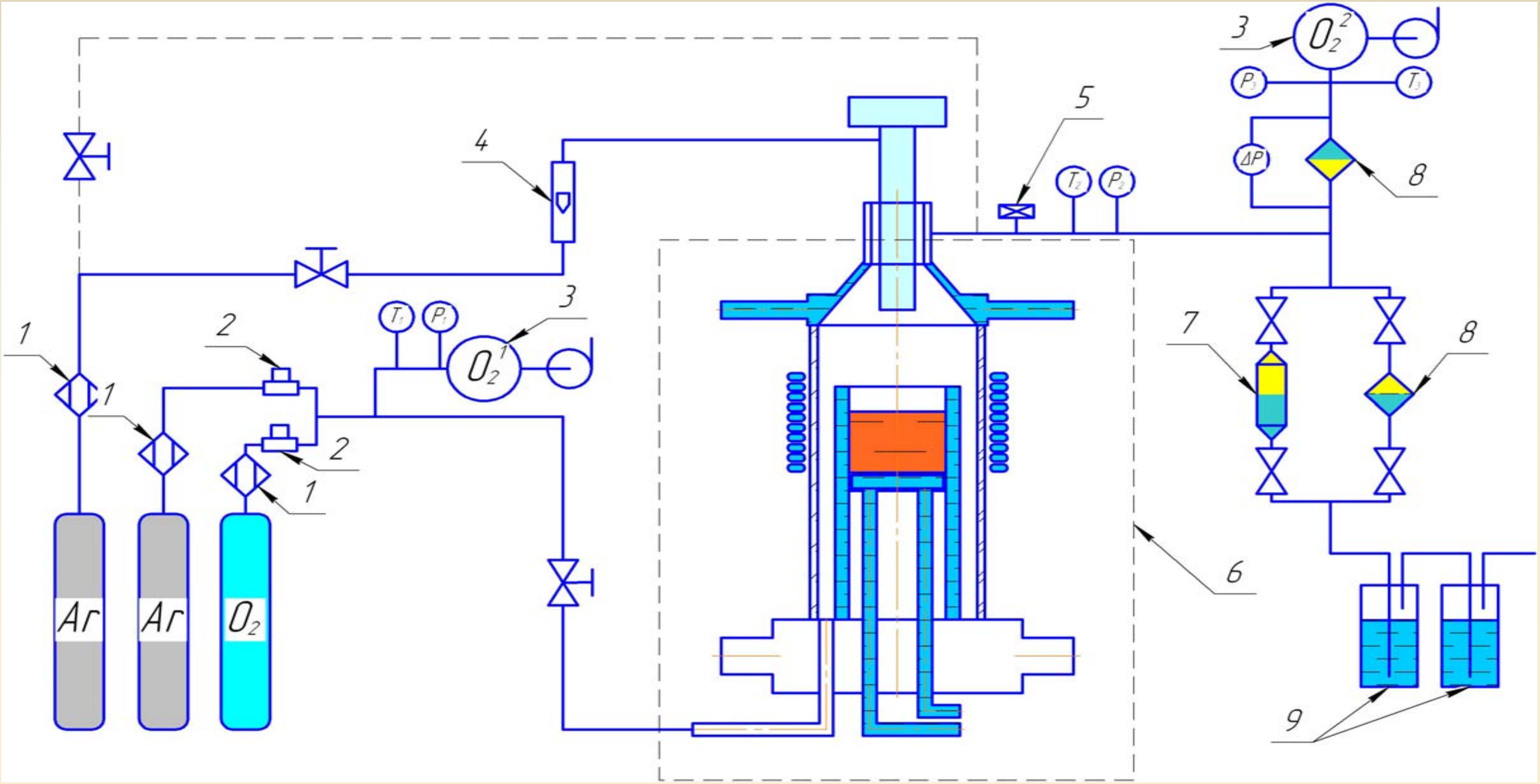


- **Transient with corium melt oxidation by Ar/O_2 mixture from C70 to C100**

1 – Main aerosol line
2 – Furnace lid
3 – Quartz tube
4 – Inductor
5 – Melt
6 – Cold crucible
7 – Bottom calorimeter
8 – Cold crucible manifold

WP2: Experiment EVAN-FP1

Gas/aerosol analytical scheme



1 –Dryer 2 – Flow controllers 3 – Oxygen sensor 4 – Flow meter 5 – Vibrator
6 – Induction furnace with cold crucible 7 – Medium area filter 8 – Analytical filters
9 – Bubblers for Ru absorption P – Pressure meters, T – Thermocouples type L

WP2: Experiment EVAN-FP1

Charge composition

Component	Component content in molten corium at VVER-1000 severe accident, mass %	Component content in charge, mass %
UO_2	76.268	72.64
ZrO_2	9.375	19.38
Zr	12.5	6.15
SrO	0.139	0.14
CeO_2	0.461	0.45
BaO	0.236	0.23
La_2O_3	0.202	0.20
Ru	0.352	0.35
Mo	0.469	0.46

WP2: Experiment EVAN-FP1

Main parameters of melt

- Melt mass: 1800 g
- Initial index of corium oxidation: C-70
- U/Zr = 1.2
- Melt temperature: 2560ºC

Above-melt atmosphere

- dry, high-purity Ar
- Argon/oxygen mixtures with O_2 volume fraction 5…20 vol. %

WP2: Modeling of fission product release from molten corium for pretest estimations

- **Development and realization of model**
  - –**thermodynamic model of system based on U-Zr - Fe – O**
  - –**evaporation rate – Langmuir equation:**

$$V = 44.44\cdot\ \bar{p}_k\ (\mathrm{atm.}) \cdot \beta_k \cdot (M_k/T)^{0.5},\ \mathrm{g/cm^2{*}\ s}$$

$$RT\ln a_k = RT\ln x_k + \sum_{j\neq k}^{n} L_{kj}\cdot x_j\cdot(1-x_k) - 0.5\sum_{i\neq k}^{n}\sum_{j\neq k}^{n} L_{ij}\cdot x_i\cdot x_j$$

- **Estimate of parameters characterizing interaction of oxygen with fission products – series of STFM-FP tests according to program "Masca" – for system U-Zr-Ru-O**

$L_{U\text{-}Zr} = 19075$

$L_{U\text{-}Ru} = 8200$

$L_{U\text{-}O} = -\ 9180$

$L_{Zr\text{-}Ru} = 19960$

$L_{Zr\text{-}O} = -\ 42470$

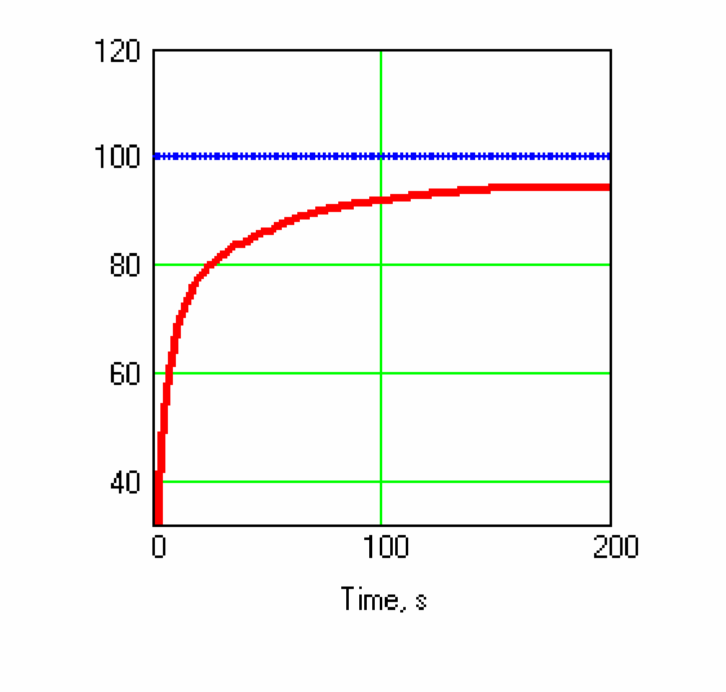
$L_{Ru\text{-}O} = 224900$

- **Example: Ru release from molten C-32 corium with atomic ratio U/Zr=0.9:**

$$V_{Ru} = 3.5\cdot10^{-7}\ \mathrm{g/cm^2}\ \cdot\mathrm{s}$$

Assessment of oxidation rate by “as it is” SOCRAT models

- **Account for Oxygen convection in the melt**
- **Unlimited oxygen at melt boundary**
- **Oxygen rate 10 l/min – total sample oxidation for 3 min**
- **At experimental values 1,2,5,10, 20 % vol – melt oxidation will be controlled by amount of available oxygen**

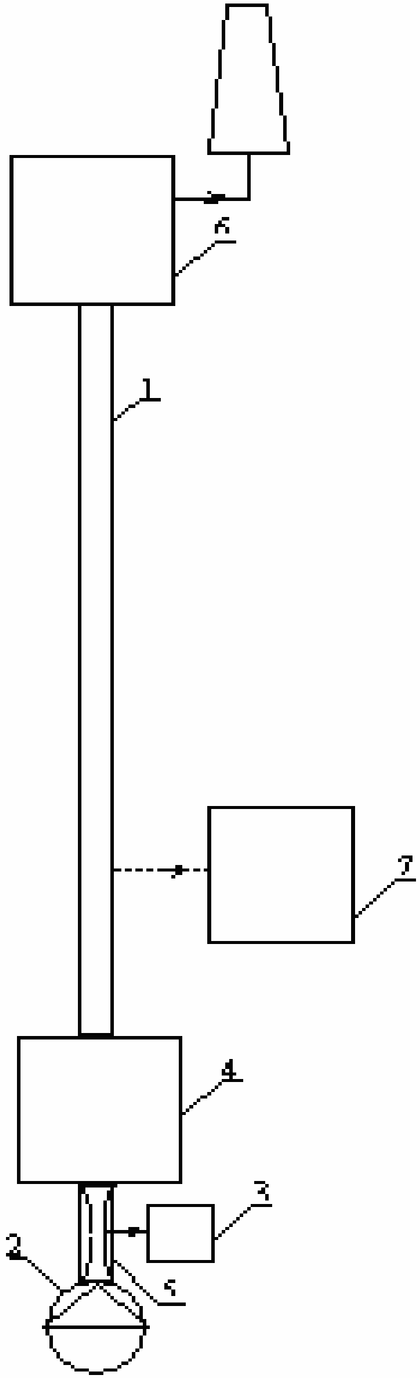


Melt Oxidation Status

WP3: Aerosol characteristic

Aerosol diameter, μm	**Aerosol generation, g/s**	**Carrier gas flow rate, m/s**	**Concentration, g/m³**
0,1-10 (at primary circuit)	100-300 (at Zr oxidation)	In reactor – up to 10 In pipes – up to 100 and higher	1-10 (at maximum release)

WP3: Experiment A1-10



Test objectives:

- Study of turbulent deposition

Facility scheme:

1 – Working section;
2 – Ventilator;
3 – Aerosol generator;
4 – Aerosol sizer;
5 – Mixing chamber;
6 – Aerosol neutralization system;
7 – Automated data gathering and processing system.

WP3: Pretest Analysis

Input data for calculations:

✓Straight pipe: 6.2 m in length; 0.098 m in diameter

✓ Isothermal conditions

✓ Range of gas rate: 0.5–100 m/s

✓ Flow mode – turbulent

✓ Particle flow – monodispersed

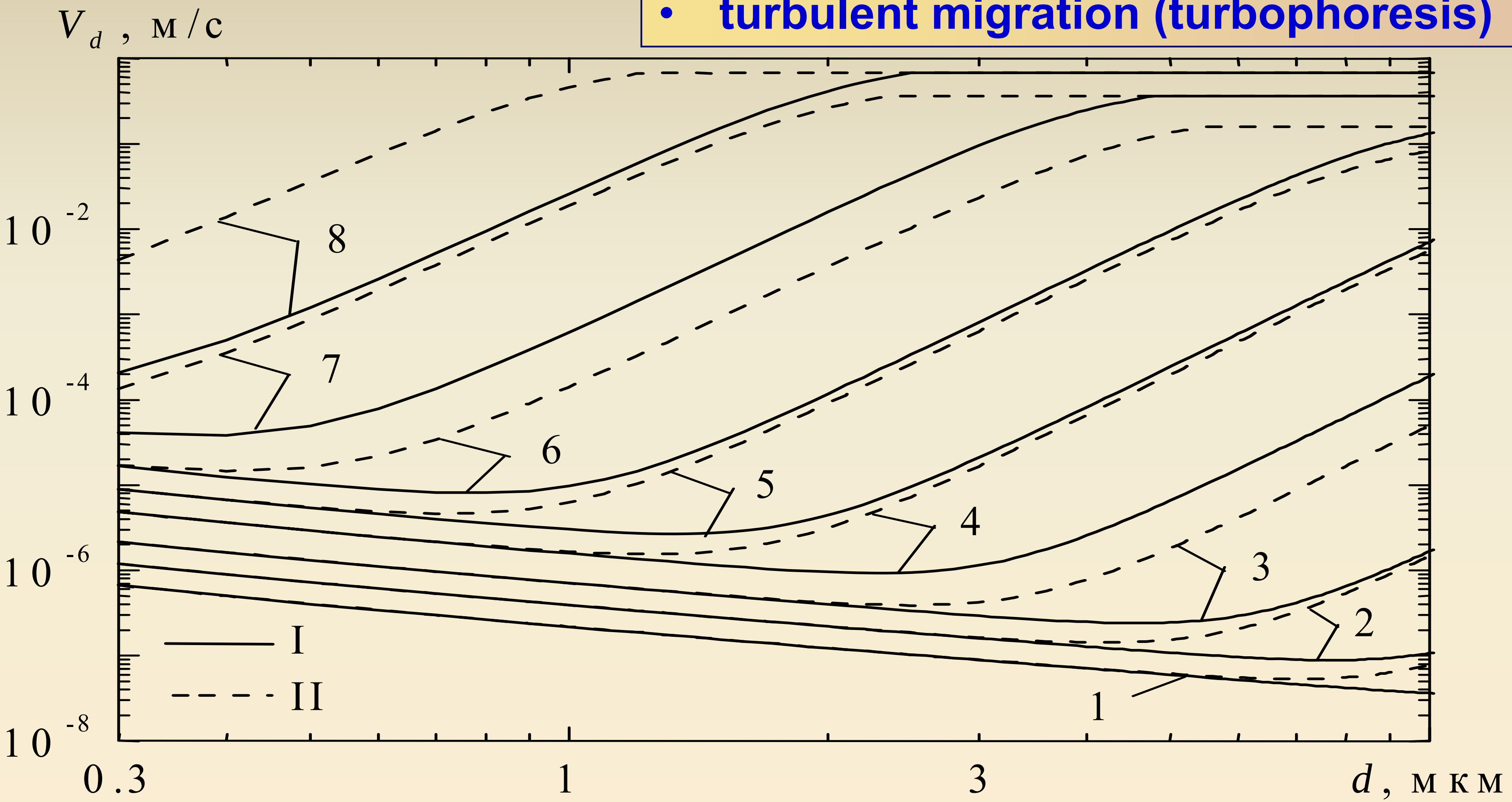
✓ Size range: 0.3–10 μm

✓ Particle density range: 1000–4000 kg/m^3

Modelling by SOKRAT/PROFIT code

Basic deposition mechanisms

- turbulent diffusion
- turbulent migration (turbophoresis)



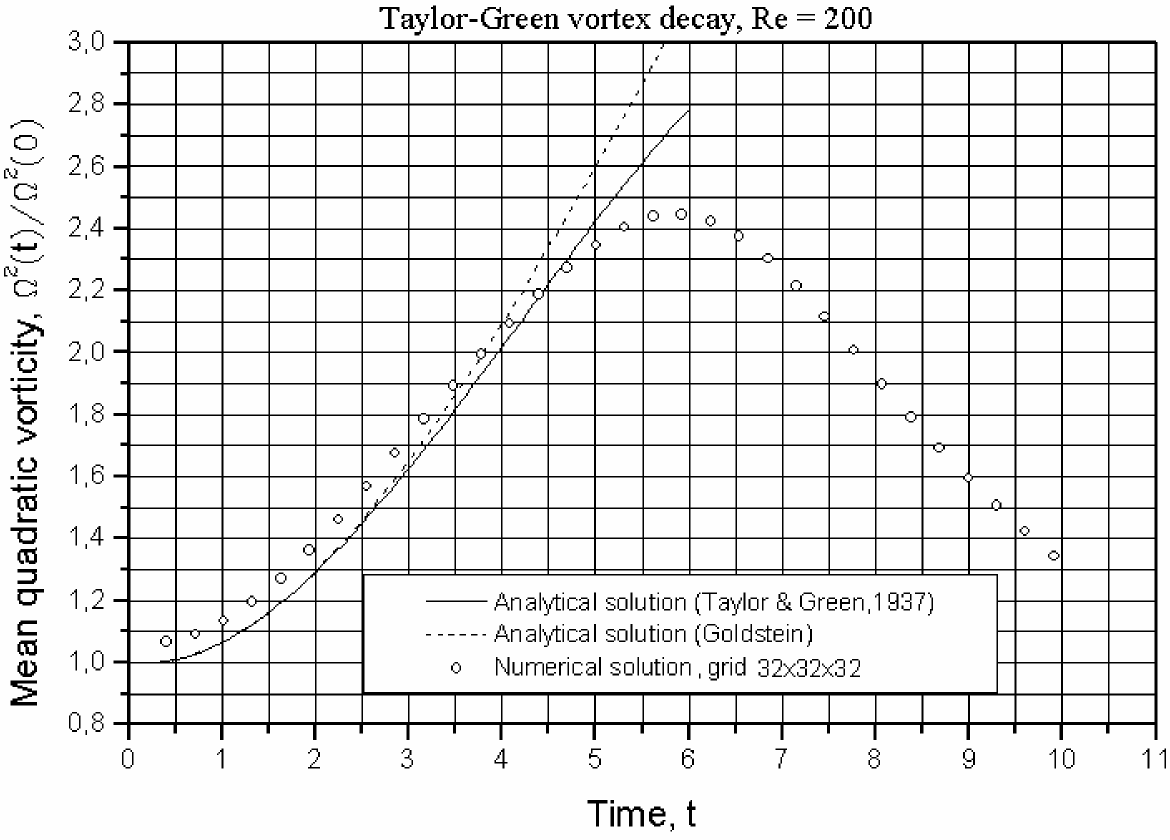
Deposition rate (m/s) versus particle diameter (µm)

Densities: **I** =1000 kg/m^3, **II** – 4000 kg/m^3;

Flow rates: 1 – 0.5 m/s, 2 – 1 m/s, 3 – 2 m/s, 4 – 5 m/s,
5 – 10 m/s, 6 – 20 m/s, 7 – 50 m/s, 8 – 100 m/s

WP3: Preparation of LES code

- Implemention of particle model
- Adaptation of code for calculation in cylindrical coordinates
- Comparison of numerical solution with analytical and verification



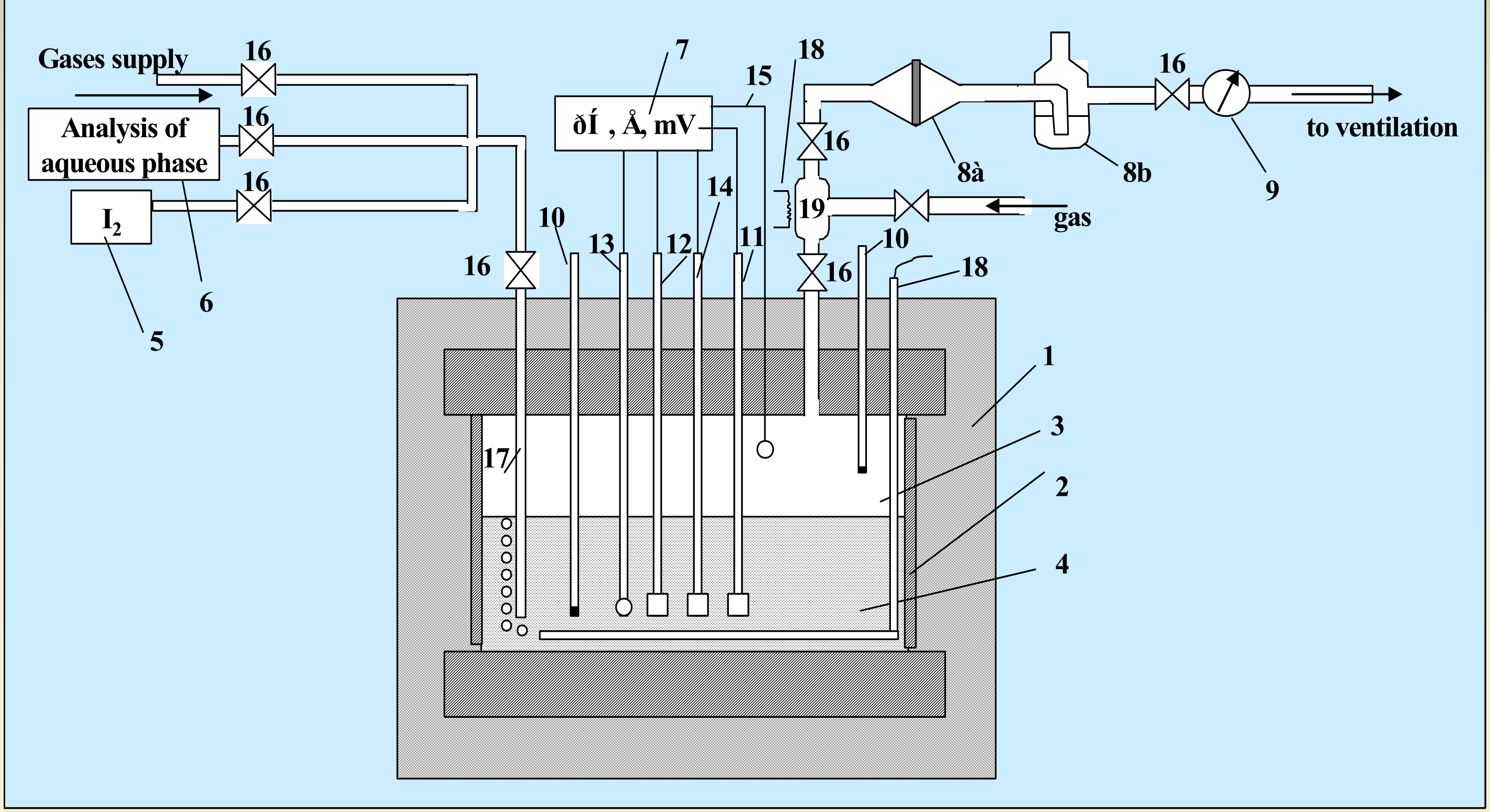
WP4: Contaiment and sump parameters typical for severe accident of VVER-1000

Concentration of H_3BO_3 in water pool, g/l	Temperature, C	pH	Doze rate / (integral doze)
15-16	up to 160	4 (no maintenance of pH) 7-8 (with maintenance of pH during severe accident)	2,2- 67 kGy/h in first day (up to 500 kGy per 30 days)

WP4: Parameters of coolants and spray solution

				Concentration				
Medium, solution	**Weight (t)**	**pH**	**H_3BO_3 (g/l)**	**Alkali metals $K^+ + Li^+ + Na^+$ (mg-equ./l)**	**NH_3, (mg/kg)**	**Cl^- (mg/kg)**	**Fe (mg/kg)**	**$N_2H_4^*$ H_2O**
Primary coolant	**240**	**5.8-10.3**	**0-16**	**0.50 ($K^+ + Li^+ + Na^+$ mg-equ./l)**	**5.0**	**0.1**	**0.05**	**-**
ECCS hydrotanks	**200**	**6.5**	**16.0**	**0.1-0.2 (only K^+ g/l)**	**-**	**-**	**-**	**200 mg/kg**
Borated water tanks	**1800**	**4.2**	**16.0**	**-**	**-**	**0.15**	**-**	**-**
Boric acid alkali solution tanks	**30**		**40**	**100-150 (only K^+ g/l)**	**-**	**-**	**-**	**200-300 mg/kg**

WP4: Experimental Study of Iodine Partitioning between Water and Gas



1 - thermostat (20-150 ^{o}C); 2 – autoclave (Teflon); 3 – gas phase; 4 – aqueous solution (I^{-}); 5 – iodine source; 6 – iodine concentration and species analysis in the aqueous phase; 7 – pH, potential and pI measuring instrument; 8 –iodine species separation in gas samples: 8a – adsorbing filters (or sorbents); 8b – barbateur; 9 – water-jet pump; 10 - thermocouple; 11 – platinum electrode; 12 – compared electrode; 13 – glass electrode; 14 – iodide-selective electrode; 15 – iodine sensor; 16 – locked tap; 17 – line of solution sampling or vapour I$_2$ (gas) supply; 18 – heater; 19 – gas sample volume measuring

WP4: Scope of work for test preparation

- **Autoclave was prepared for research of iodine water/gas partition in presence of sorbent -ferric hydroxide.**
- **Methodics were developed for analysis of iodine concentration in samples of water/gas phases.**
- **Ferric hydroxides were prepared by its precipitation in solution of ferric chloride or ferric nitrate.**
- **The iron concentration and characteristics of ferric hydroxides were determinated.**

WP4: Modelling

- Kinetic model has been developed for calculating the distribution of iodine forms among aqueous and gaseous phases
- The model is a system of equations describing water radiolysis, iodine hydrolysis reactions, interaction of iodine forms with water radiolysis products and organic impurities, iodine sorption on equipment and containment surfaces, mass exchange between aqueous and gaseous phases
- The code is structured as a four-block tool: aqueous phase, gaseous phase, sorption/desorption on surfaces, pH calculation.
- The database contains 42 reactions: 20 iodine reactions include 10 iodine forms,14 reactions of 8 boron and ammonia forms, 4 reactions with iron ions and 4 reactions with three organic forms of iodine.

WP4: Modelling (2)

- The radiolysis block contains system of equation for water radiolysis.
- 1st version of iodine module has been prepared. This version can take into account influence of impurities (NH3 and products of ammonia radiolysis, H3BO3, Fe3+, CH4) and iodine sorption on polymeric coating. As the main source of volatile forms of iodine in the containment atmosphere is mass exchange between aqueous and gaseous phases, and most of iodine is removed from water due to sorption in aqueous phase, changing of the rate constants for these processes is critical.
- Adapted iodine model and calculation code are used in pretest calculations for WP4

Modelling: Constants of radiolytic and chemical reactions

No.	Reaction	Rate constant k_{298} (l/mol·s)	Activation energy E_a (kJ/mol)
1	$I_2+H_2O\rightarrow I_2OH^-+H^+$	$1.0\cdot10^{10}$	12.5
2	$I_2OH^-+H^+\rightarrow I_2+H_2O$	$3.0\cdot10^{10}$	-
3	$I_2OH^-\rightarrow HOI+I^-$	$1\cdot10^{6}$	-
4	$HOI+I^-\rightarrow I_2OH^-$	$6.1\cdot10^{2}$	-
5	$2HOI\rightarrow IO_2^-+I^-+2H^+$	$.34\cdot10^{6}$	-
6	$IO_2^-+I^-+2H^+\rightarrow 2HOI$	$1.7\cdot10^{10}$	-
7	$HOI+IO_2^-\rightarrow IO_3^-+I^-+H^+$	$1.0\cdot10^{7}$	-
8	$IO_3^-+I^-+H^+\rightarrow HOI+IO_2^-$	0.58	-
9	$2I\rightarrow I_2$	$1.0\cdot10^{10}$	-
10	$I_2+OH_2^-\rightarrow HOOI+I^-$	$4.0\cdot10^{8}$	16.0
11	$HOI+I^-\rightarrow I_2+HO_2^-$	$5.0\cdot10^{5}$	16.0
12	$HOI+HO_2^-\rightarrow HOOI+OH^-$	$2.1\cdot10^{9}$	16.0
13	$HOOI+OH^-\rightarrow I_2^-+O_2+H_2O$	$2.0\cdot10^{9}$	16.0
14	$I_2+O_2^-\rightarrow I_2^-+O_2$	$3.9\cdot10^{9}$	6.7
15	$H_3BO_3+H_2O\rightarrow H^++H_4BO_4^-$	$8.11\cdot10^{1}$	7.6
16	$H^++H_4BO_4^-\rightarrow H_3BO_3+H_2O$	$1.4\cdot10^{11}$	12.6
17	$NH_3+H_2O\rightarrow NH_4^++OH^-$	$5.94\cdot10^{5}$	(to be determined)
18	$NH_4^++OH^-\rightarrow NH_3+H_2O$	$3.3\cdot10^{10}$	12.6
19	$NH_4^++e^-_{aq}\rightarrow NH_3+H$	$1.7\cdot10^{6}$	20.93
20	$NH_3+OH\rightarrow NH_2+H_2O$	$9.0\cdot10^{7}$	13.94

Modelling: Constants of radiolytic and chemical reactions (2)

21	$NH_3+H \rightarrow NH_2+H_2$	$1,1 \cdot 10^1$	13,94
22	$NH_2+H_2O_2 \rightarrow H_2O+NHOH$	$9,0 \cdot 10^7$	13,94
23	$NH_2+HO_2 \rightarrow O_2+NH_3$	$1,0 \cdot 10^{10}$	12,6
24	$NH_2+O_2^- \rightarrow O_2+NH_3+OH^-$	$1,0 \cdot 10^{10}$	12,6
25	$NH_2+H \rightarrow NH_3$	$1,0 \cdot 10^{10}$	12,6
26	$NH_2+e^-_{aq} \rightarrow NH_3+ OH^-$	$1,0 \cdot 10^{10}$	12,6
27	$2NHOH \rightarrow N_2+2H_2O$	$1,0 \cdot 10^{10}$	12,6
28	$NH_2+NHOH \rightarrow N_2+H_2+H_2O$	$1,0 \cdot 10^{10}$	12,6
29	$Fe^{3+}+e_{aq}^- \rightarrow Fe^{2+}+H_2O$	$2,3 \cdot 10^{10}$	12,6
30	$Fe^{3+}+H \rightarrow Fe^{2+}+H^+$	$9,6 \cdot 10^7$	12,6
31	$Fe^{2+}+OH \rightarrow Fe^{3+}+OH^-$	$3,0 \cdot 10^8$	12,6
32	$Fe^{2+}+HO_2 \rightarrow Fe^{3+}+HO_2^-$	$3,0 \cdot 10^7$	12,6
33	$CH_4+OH \rightarrow CH_3+H_2O$	$1,21 \cdot 10^8$	—
34	$CH_3+I_2 \rightarrow CH_3I+I$	$6,0 \cdot 10^9$	—
35	$CH_3I+e_{aq}^- \rightarrow CH_3+I^-$	$1,6 \cdot 10^{10}$	—
36	$CH_3I+H \rightarrow CH_3+H^++I^-$	$1,0 \cdot 10^{10}$	—
37	$HOI \rightarrow H^++IO^-$	0,1	—
38	$H^++IO^- \rightarrow HOI$	$1,0 \cdot 10^{10}$	—
39	$I_2+I^- \rightarrow I_3^-$	$4.5 \cdot 10^9$	—
40	$I_3^- \rightarrow I_2+I^-$	$7,5 \cdot 10^6$	—
41	$HOI^- + I \rightarrow I_2 + OH^-$	$2,3 \cdot 10^{10}$	—
42	$2HOI^- \rightarrow I_2 + 2OH^-$	$2,0 \cdot 10^{10}$	—

WP4: Input data for pretest calculations

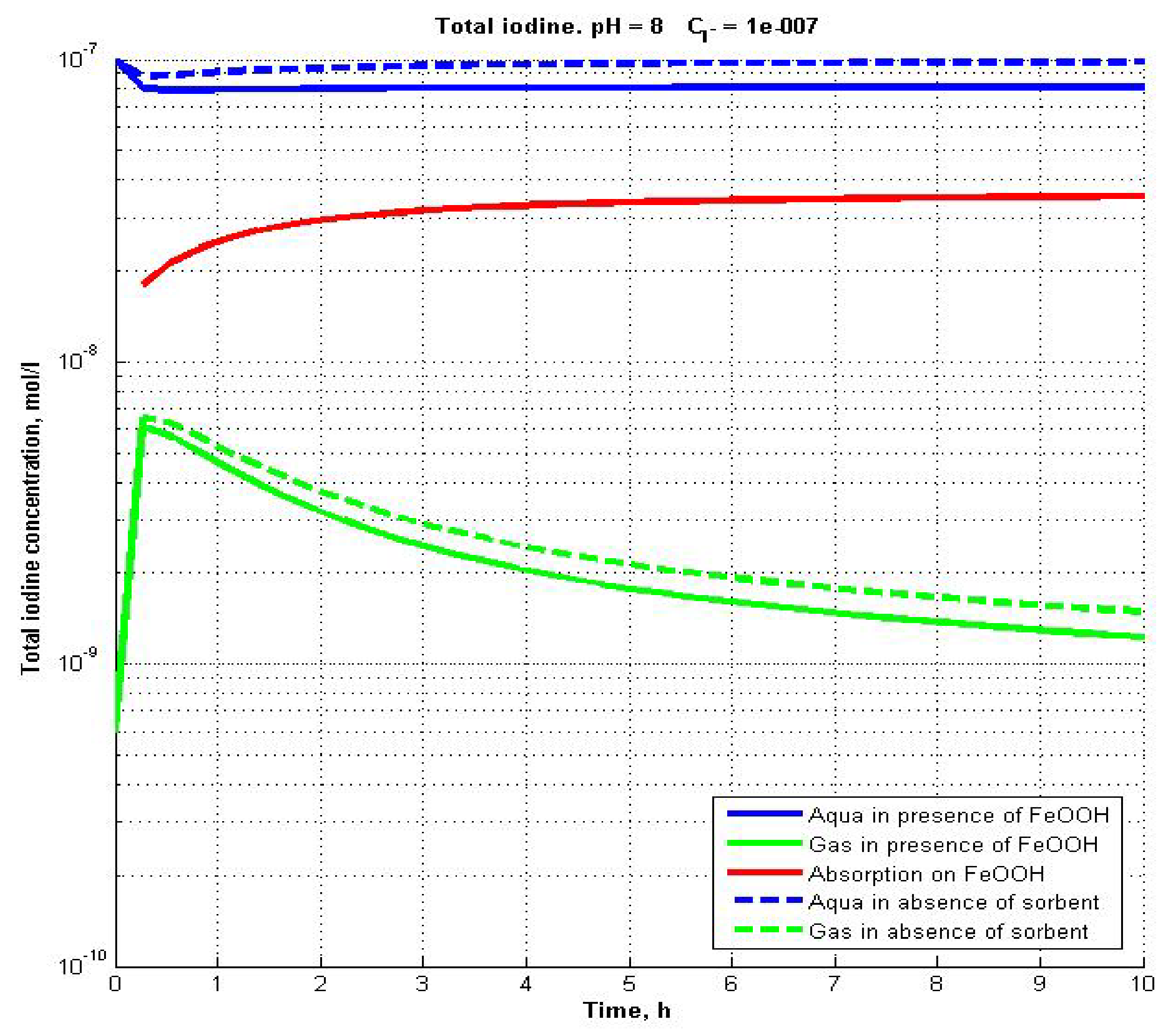
Pretest calculations of volatile iodine forms (I_2, I) concentration in gas phase were carried out with consideration of iodine forms adsorption on ferric hydroxide.

Ampule test conditions:

- Composition of aqueous solution: 1e-005-1e-007 mol/l Cs(K)I + 10 g/l boric acid.
- Temperature – 25 C
- Dose rate – 1 kGy/h, integral dose – 10 kGy.
- Initial iodide-ion concentration in water, mol/l: 1e-005; 1e-007;
- pH: 4; 6,5; 8;
- FeOOH concentration, g/l: 0; 2,5.

! Presence of organic impurities and iodine adsorption on inner ampule surfaces doesn’t accounted in calculations.

WP4: Results of pretest calculations
Iodine consentrations(mol/l) versus time (h). pH=8



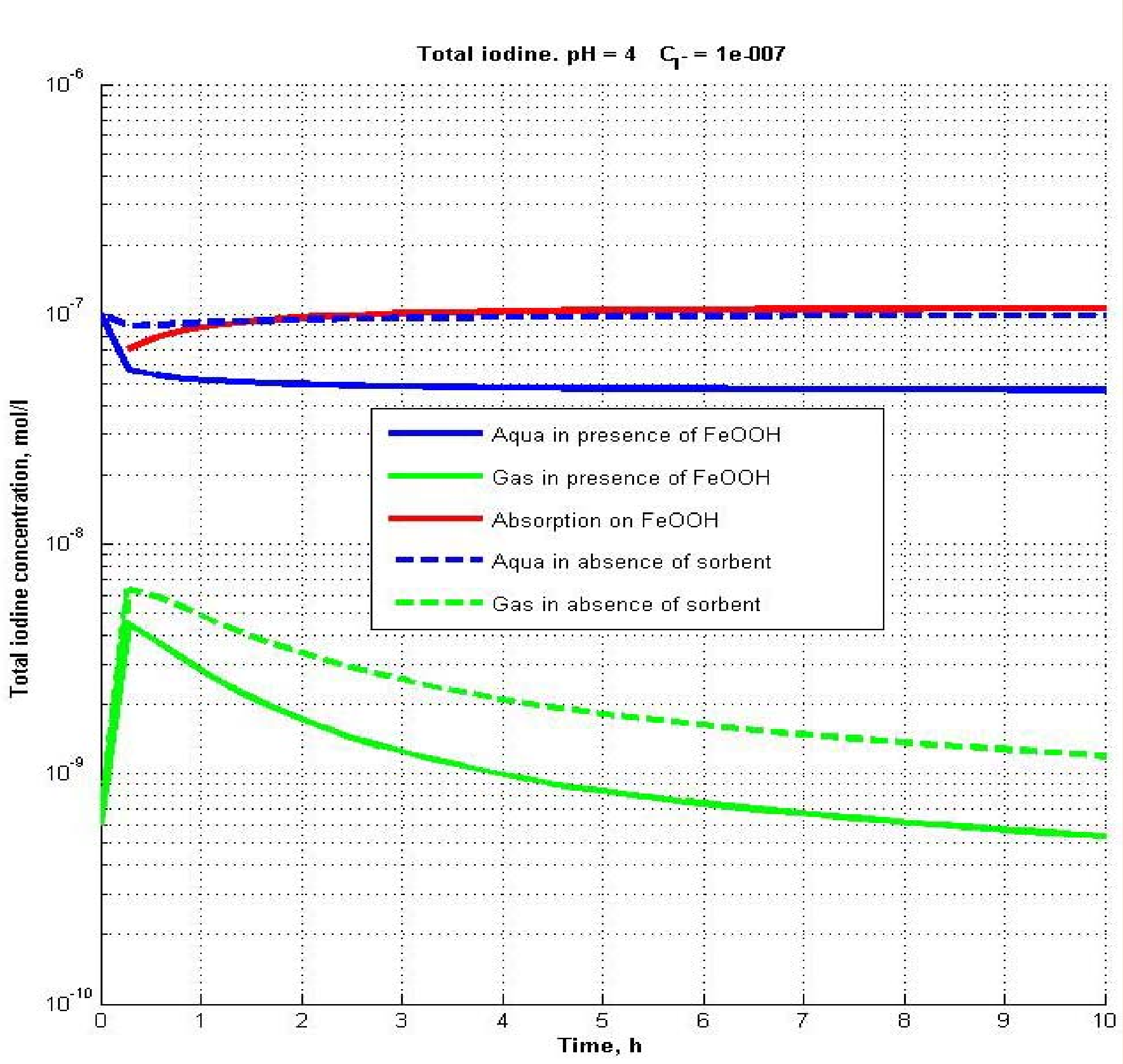
Iodine volatile forms concentration in gas phase in presence or absence of sorbent (FeOOH); pH=8

- **Iodide-ion concentration in water solution=1e-007.**

- **Iodide adsorption = ~35%.**

- **Iodide-ion adsorption on ferric hydroxide doesn't much influence on iodine volatility at low iodide concentration in water solutions and pH=8.**

WP4: Results of pretest calculations
Iodine consentrations(mol/l) versus time (h). pH=4



Iodine volatile forms concentration in gas phase in presence or absence of sorbent (FeOOH); pH=4

- **Iodide concentration in**
- **water solution = 1e-007 mol/l.**

- **Iodide-ion adsorption on FeOOH =~95%.**

- **At low pH and iodide-ion concentration in adsorbent presence**

- **Iodine volatile species release is reduced in 2,5-3 time.**

CONCLUSIONS

- **Analysis of VVER-1000 scenarios provided conditions of experiments of WP2, 3, 4**
- **Conceptual design of test facilities have been done on the base of pretest calculations**
- **The planned tests will be descussed with collaborators at the 1st project meeting. Meeting dates will be coordinated by e-mail.**