SOME CONSIDERATIONS ON THE SCALING OF EXPERIMENTS FOR HYDROGEN RISK ASSESSMENT

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ABSTRACT

Experimental facilities for the safety analysis of nuclear systems and new technologies, having hydrogen safety as the main subject of research, have been operated since several years at the CEA (Commissariat à l'Energie Atomique).

It is well known that, for practical reasons, experimental investigation on hydrogen safety issues often adopts mixtures of different gases. Helium is commonly used as a substitute for hydrogen.

This paper deals with the phenomenological analysis of light gas dispersion phenomena of interest in the field of hydrogen safety.

First, a simple analytical methodology is proposed to identify the relevant parameters in a diffuse leak scenario and to guide the scaling of experiments using helium as a substitute for hydrogen.

Involving typical scales of the experiments performed at the CEA/LEEF, examples of applications of this methodology are then proposed.

In one of the considered cases, it is also demonstrated that the dynamic phenomena involved in the dispersion of a cloud of hydrogen are of the same order than in a cloud of helium having the same molar concentration.

Nomenclature

$\mathcal{D}$	Binary diffusion coefficient	ρ	Density
(δp)	Pressure scale	Re	Reynolds number
ϵ	Dilatation factor	Ri	Richardson number
Fr	Froude number	Sc	Schmidt number
g	Acceleration of gravity (9.81m/s^2)	St	Strouhal number
$\hat{k}$	Vertical unity vector	t	Time
L	Length scale	τ	Time scale
μ	Dynamic viscosity	$\vec{v}$	Velocity
ν	Kinematic viscosity	V	Velocity scale
p	Pressure	Y	Transported mass fraction
Pe	Péclet number		

Subscripts

0	Refers to initial conditions	d	Refers to diffusion
∞	Refers to far-fields conditions	ref	Generic reference conditions
c	Refers to convection		

1 Introduction

Safety of technological applications concerns the whole life cycle of a product: the design, the type-approval, the production, the operation and the disposal. Vendors and manufacturers are often due to produce evidences of it [1, 2].

An extensive R&D work, including both experimental and modeling activities is sometimes essential to perform the required safety and risk analysis. Experiments can be used also to provide databases for the validation of mathematical and numerical models.

As the set-up of a full scale arrangement is rarely convenient, scaling is often adopted in the aim of reducing costs and delays of the experimental activities. In these cases, the biases due to scale distortions need to be clearly identified and quantified. Indeed, top-down analysis of complicated processes may require some separated effects experiments [3]. Several scaled experiments can be therefore necessary to address a single specific problem [4].

When very complicated systems are concerned, a qualified pool of experts may take several years of research to define the appropriate scaling strategy for the experimental campaign [5]. Then, the system is decomposed and each experiment addresses only a part of it.

For practical and operational reasons, mixture of other non flammable gases are often used to address hydrogen safety issues [6]. Helium is sometimes used as a convenient substitute for hydrogen, since its behaviour is supposed to be similar because of its similar physical properties. However, it is not always clear on which basis, and to what extent, the suitability of helium is assessed [7, 8].

At the CEA/LEEF (Experimental Fluid Mechanics Laboratory), the MISTRA facility has been operated since the 90s to investigate the thermal-hydraulic behaviour of light water nuclear reactor containments under postulated accidental conditions [9]. GAMELAN and GADIFFAN are separate effect facilities conceived to analyze thermal-hydraulic phenomena at smaller scales [10]. The GARAGE facility has been conceived to provide experimental data that are considered to be representative of an hypothetic leak caused by an hydrogen system in a full scale private garage [11].

This article addresses a simplified analysis of hydrogen dispersion and dilution, that is the case of a diffuse leak. When a fluid is released in an obstructed medium of different density and its momentum is rapidly dissipated, a diluted cloud containing the released and the surrounding fluids establishes. Then, due to buoyancy forces, the cloud starts to flow as a buoyant thermal [12].

A phenomenological analysis of the early phase of the dispersion is proposed, on whose basis it is thus be possible to determine the relevant mechanisms as well as the corresponding time and velocity scales. Therefore, some examples of the application of this methodology are reported for small and large scale facilities and a comparison between an air-hydrogen and an air-helium mixture is proposed.

2 Free convection in binary mixtures

The non-reactive transport of a chemical species can be promoted by molecular diffusion as well as advection. The term *convection* generally refers to those situations where the flow rises from externally induced temperature variations. Nevertheless, flows with concentration variations may be treated in the same way. Therefore, the denomination of *convection* is used in these cases as well [13].

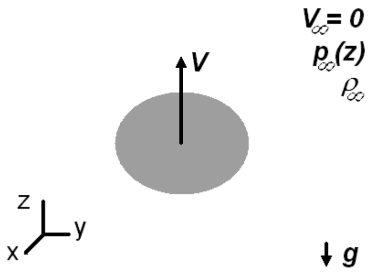

Figure 1: Case sketch.

2.1 Governing equations

Let's consider a fluid cloud of a generic shape (but without any preferred directions), with initial uniform mass fraction Y_0 (figure 1). The balance equations for mass, momentum and transported chemical species are respectively [13]:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \rho \vec{v} = 0 \tag{1}$$

$$\rho \frac{\partial \vec{v}}{\partial t} + \vec{\nabla} \vec{v} \cdot \rho \vec{v} = \vec{\nabla} \cdot \mu \vec{\nabla} \vec{v} - \vec{\nabla} p + \rho \vec{g} \tag{2}$$

$$\rho \frac{\partial Y}{\partial t} + \rho \vec{v} \cdot \vec{\nabla} Y = \vec{\nabla} \cdot (\rho \mathcal{D} \vec{\nabla} Y) \tag{3}$$

Let us assume that the mixture density depends only on the species concentration. ($\rho = \rho(Y)$). If the variations of Y around a reference condition Y_{ref} are small (figure 2), it is possible to use an affine expression to put the mass fraction in a dimensionless form ($Y = Y_{\text{ref}} + (Y_0 - Y_{\text{ref}})Y^*$). The equation of state can be then linearized by using a Taylor series. In our case of hydrogen dilution, the concentration of the transported species is considered to be zero in the far field ($Y_{\text{ref}} = Y_\infty = 0$) and therefore $Y = Y_0 Y^*$. Assuming that Y_0 is small, the equation of state can be linearized by using the Mc Laurin series:

$$\rho = \rho_\infty (1 - \epsilon Y^*) \tag{4}$$

where $\epsilon = -\frac{Y_0}{\rho_\infty} \frac{\partial \rho}{\partial Y}|_{Y_\infty = 0}$.

To turn the balance equations in the dimensionless formulation, the following normalizations are therefore introduced:

$$\begin{array}{llllll} \vec{v} = V\ \vec{v}^* & ; & t = \tau\ t^* & ; & & \\ \mu = \mu_\infty\ \mu^* & ; & p = P_\infty - \rho_\infty g z + (\delta p) p^* & ; & & \\ \vec{\nabla} \circ = \frac{1}{L} \nabla^* \circ & ; & \Delta \circ = \frac{1}{L^2} \Delta^* \circ & ; & \frac{\partial}{\partial t} \circ = \frac{1}{\tau} \frac{\partial}{\partial t^*} \circ \end{array} \tag{5}$$

In a general three dimensional case without preferential directions, a unique length scale L and a unique velocity scale V can be retained for the three directions. Implicitly assuming that the surrounding geometry does not affect the shape of the cloud, the length scale L accounts for its dimension.

According to the previous normalizations, the dimensionless balance equations can be written as:

$$\vec{\nabla}^* \cdot \vec{v}^* = \frac{\epsilon L}{V \tau} \frac{\partial Y^*}{\partial t^*} + \epsilon \vec{v}^* \cdot \vec{\nabla}^* Y^* \tag{6}$$

$$\frac{L}{V \tau} \frac{\partial \vec{v}^*}{\partial t^*} + \vec{v}^* \cdot \vec{\nabla}^* \vec{v}^* = \frac{\nu_\infty}{V L} \vec{\nabla}^* \cdot \mu^* \vec{\nabla}^* \vec{v}^* - \frac{(\delta p)}{\rho_0 V^2} \vec{\nabla}^* p^* + \frac{g L}{V^2} \epsilon Y^* \hat{k} \tag{7}$$

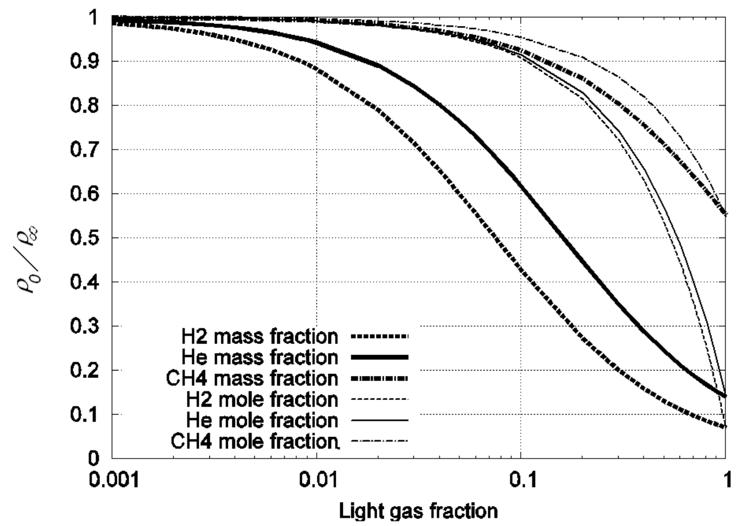

Figure 2: Initial conditions as a function of the light gas type and concentration, expressed in terms of mass fraction (bold lines) and mole fraction (thin lines).

$$\frac{L}{V\tau}\frac{\partial Y^*}{\partial t^*} + \vec{v}^* \cdot \vec{\nabla}^* Y^* = \frac{\mathcal{D}}{VL}\Delta^* Y^* \tag{8}$$

where the molecular diffusion coefficient $\mathcal{D}$ is assumed to be constant in the species balance equation.

Boundary conditions are assigned to the surrounding atmosphere. The released fluid is assumed to be absent in the far-field region ($Y^* = 0$) whereas the pressure p_∞ depends on the z coordinate ($p_\infty = p(z)$). Besides, the surrounding atmosphere is assumed to be stagnant. Initial conditions are assigned to the cloud, where $Y^* = 1$ at the beginning of the dispersion transient.

The terms containing ϵY^* have been neglected in each dimensionless group of the balance equations, with the exception of the buoyancy force term. Of course, since buoyancy is the only cause of the flow, it can not be neglected.

The well known dimensionless numbers, namely the Froude, the Péclet, the Reynolds, the Schmidt number and the Strouhal numbers, can be recognized in the balance equations 6, 7 and 8:

$$\mathrm{Fr} = \frac{V}{\sqrt{gL}} \quad ; \quad \mathrm{Pe} = \frac{VL}{\mathcal{D}} = \mathrm{ReSc} \quad ; \quad \mathrm{Re} = \frac{VL}{\nu_\infty} \quad ; \quad \mathrm{Sc} = \frac{\nu_\infty}{\mathcal{D}} \quad ; \quad \mathrm{St} = \frac{L}{V\tau} \tag{9}$$

The Richardson number Ri is defined as ϵ/Fr^2.

2.2 Phenomenological analysis

The problem is now defined by the equations 4, 6, 7, 8 and the aforementioned boundary conditions. The unknown scales of the problem are the velocity scale, the pressure scale and the time scale.

In the momentum equation, it is not possible to neglect at the same time both the inertia and the viscous forces. As this case study concerns the buoyant flow due to natural convection, we are not interested in stagnating conditions.

The pressure gradient is consequential to the flow, and has to be retained in the momentum equation at every approximation. In this aim:

$$(\delta p) = \epsilon \rho_\infty g L \tag{10}$$

As nothing prevents mass diffusion from being faster (or slower) than the convection, two time scales need to be considered. Therefore, a convection time scale τ_c is used in the equation 7 and a diffusion time scale τ_d is used in the equation 8. The Orders of Magnitude equations are thus obtained from the balance equations:

$$1 = \sup\left\{\frac{\epsilon L}{V\tau}; \epsilon\right\} \tag{11}$$

$$\epsilon\frac{gL}{V^2} = \sup\left\{\frac{L}{V\tau_c}; 1; \frac{\nu_\infty}{VL}; \frac{(\delta p)}{\rho_\infty V^2}\right\} \tag{12}$$

$$\frac{L}{V\tau_d} = \sup\left\{1; \frac{\mathcal{D}}{VL}\right\} \tag{13}$$

The convection time scale is obtained from equation 12 equating the convection term to the buoyancy term. The diffusion time scale is obtained from equation 13 equating the diffusion term to the time variation. Namely:

$$\tau_c = \frac{V}{\epsilon g} \quad ; \quad \tau_d = \frac{L^2}{\mathcal{D}} \tag{14}$$

However, the relevant phenomenon for the early development of the cloud is the one with the shorter time scale. As the diffusion time scale is known a priori, the evaluation of the velocity scale marks out the dominating mechanism and the condition on the velocity divergence (equation 11).

The evaluation of the dominating time scale is also necessary to analize the continuity equation. In fact, when ϵ is small, one gets:

$$\frac{\epsilon L}{V\tau} \ll 1 \qquad \Longrightarrow \qquad \vec{\nabla}^* \cdot \vec{v}^* = 0 \tag{15}$$

This condition for the degeneration of the equation needs to be verified for each application.

Three different situations are now addressed:

- the viscous forces are negligible with respect to the inertia forces

$$\frac{\nu_\infty}{VL} << 1 \tag{16}$$

- the inertia forces are negligible with respect to the viscous forces

$$\frac{\nu_\infty}{VL} >> 1 \tag{17}$$

- the inertia forces and the viscous forces are of the same order

$$\frac{\nu_\infty}{VL} \sim 1 \tag{18}$$

Figure 3: Species transport in the early stage.

2.2.1 Negligible viscous forces

In the case of negligible viscous forces, the inertia forces balance the body forces. Therefore the resulting velocity scale is given by

$$\epsilon \frac{gL}{V^2} = 1 \qquad \Longrightarrow \qquad V = \sqrt{\epsilon g L} \tag{19}$$

under the condition that

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \ll 1 \tag{20}$$

The corresponding Froude and Richardson numbers are respectively: $\mathrm{Fr} = \sqrt{\epsilon}$ and $\mathrm{Ri} = 1$.

Now both the time scales of the equation 14 are known. In fact $\tau_d = L^2/\mathcal{D}$ and $\tau_c = V/\epsilon g = L/\sqrt{\epsilon g L}$.

The dominant mechanism of the species transport emerges from the comparison of the two time scales (figure 3). A a further condition on $\mathcal{D}$ can thus be found.

The convection is relevant when:

$$\tau = \tau_c \ll \tau_d \qquad \Longleftrightarrow \qquad \mathcal{D} \ll L\sqrt{\epsilon g L} \tag{21}$$

The relevant time scale in this case is $\tau = \tau_c$. Therefore, the Péclet number is high and the species equation degenerates in an advection equation: the cloud starts to float up and retains sharp concentration gradients. Moreover, the condition of equation 15 is satisfied and it is possible to assume $\vec{\nabla}^* \cdot \vec{v}^* = 0$.

On the other hand, a mainly diffusive transport occurs in case of very high diffusivities or relating to very small cloud. As a result, the concentration gradients quickly smooth. It happens when:

$$\tau = \tau_d \ll \tau_c \qquad \Longleftrightarrow \qquad \mathcal{D} \gg L\sqrt{\epsilon g L} \tag{22}$$

With this time scale the condition of equation 15 is not satisfied, and the continuity equation should be used in the form of the equation 6.

Finally, if $\tau_c \sim \tau_d$, both advection and diffusion transport processes concur to transport the released fluid. The condition of equation 15 needs to be checked.

2.2.2 Dominant viscous forces

In the case of negligible inertia forces, the viscous forces balance the body forces. The velocity scale is given by

$$\epsilon \frac{gL}{V^2} = \frac{\nu_\infty}{VL} \qquad \Longrightarrow \qquad V = \frac{\epsilon g L^2}{\nu_\infty} \tag{23}$$

under the condition that:

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \gg 1 \tag{24}$$

The Froude number is $\mathrm{Fr} = \epsilon L\sqrt{gL}/\nu_\infty$ and the Richardson number is $\mathrm{Ri} = \nu_\infty^2/(\epsilon g L^3)$. The two time scales are thus $\tau_c = V/\epsilon g = L^2/\nu_\infty$ and $\tau_d = L^2/\mathcal{D}$.

As in the previous case, for low values of the Péclet number, the species equation degenerates in an advection one. Namely, if

$$\tau = \tau_c \ll \tau_d \qquad \Longleftrightarrow \qquad \mathcal{D} \ll \nu_\infty \tag{25}$$

the cloud floats up without dissipating the sharp concentration gradient. Using the appropriate values for the velocity and the convection time scale, the equation 15 gives that:

$$\vec{\nabla}^* \cdot \vec{v}^* = 0 \qquad \Longleftrightarrow \qquad \frac{\nu_\infty^2}{gL^3} \ll 1 \tag{26}$$

On the contrary, when

$$\tau = \tau_d \ll \tau_c \qquad \Longleftrightarrow \qquad \mathcal{D} \gg \nu_\infty \tag{27}$$

a mainly diffusive transport establishes and the concentration gradients quickly smooth. The velocity and the diffusion time scales should be then used in the equation 15 to get:

$$\vec{\nabla}^* \cdot \vec{v}^* = 0 \qquad \Longleftrightarrow \qquad \frac{\nu_\infty \mathcal{D}}{gL^3} \ll 1 \tag{28}$$

Finally, when $\mathcal{D} \sim L\sqrt{\epsilon g L}$, both advection and diffusion concur to transport the released fluid, and the degeneration of the continuity equation 6 needs to be checked.

2.2.3 Full momentum transport

When:

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \sim 1 \tag{29}$$

the viscous forces and the inertia forces are of the same order.

In this case, the full momentum transport is to be considered, including the advective term (the inertia forces) and the diffusive term (the viscous forces). The velocity scale is $V = \sqrt{\epsilon g L} = \nu_\infty/L$ and the time scales are: $\tau_c = L/\sqrt{\epsilon g L} = L^2/\nu_\infty$ and $\tau_d = L^2/\mathcal{D}$.

Depending on the Péclet number or, as $\mathrm{Re} \sim 1$, on the Schmidt number (i.e. on the considered species), the analysis of the species transport can lead to a degenerated problem in terms either of advective or diffusive transport. The degeneration of the continuity equation should be discussed in both cases.

3 Applications of the methodology

In this section, the methodology that we have illustrated in the previous paragraph is applied to scenarios having different length and buoyancy scales.

At the Experimental Fluid Mechanics Laboratory (LEEF) of the CEA Saclay, the MISTRA, the GAMELAN, the GADIFFAN and the GARAGE facilities are mainly operated in the frame of research programs dealing with hydrogen safety. In all the facilities it is possible to inject different gaseous species in a confined volume and to record the

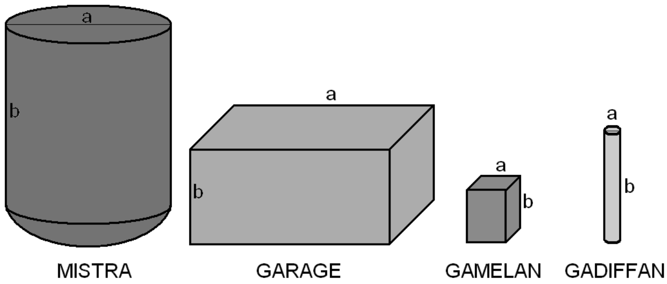

Figure 4: Facilities sketch. The lengths a and b are used in table 1 to calculate the aspect ratio.

evolution of the concentrations at several monitoring points. Therefore, the facilities can be used to address gaseous dispersion and dilution in uniform or stratified atmospheres.

The detailed descriptions of their layout, operation, aims and results are available in open literature [9, 10, 11]. For the needs of this paper, a simplified sketch is proposed in figure 4. The table 1 shows their aspect ratios and volumes. The length scales vary up to one order of magnitude.

The following analysis investigates the dispersion of a gaseous cloud at the length scales typical of GADIFFAN and MISTRA. The suitability of helium as a substitute for hydrogen is assessed for the cases at larger length scale.

It is assumed that $\nu_\infty = 1.5 \cdot 10^{-5}\text{m/s}^2$ in the far field (pure air) and that helium and hydrogen have the same molecular diffusivity in air ($\mathcal{D} = 7.4 \cdot 10^{-5}\text{m/s}^2$) [14].

Table 1: Main features of the facilities operated at LEEF.

Facility	Shape	Aspect ratio a/b	Volume
MISTRA	Cylinder	0.6	100m^3
GARAGE	Parallelepiped	2.2	40m^3
GAMELAN	Parallelepiped	0.8	1m^3
GADIFFAN	Cylinder	0.1	0.1m^3

3.1 Hydrogen dispersion at a smaller scale

A spherical cloud of hydrogen is considered, having a characteristic lenght $L = 0.1\text{m}$ (e.g. the diameter). Let the initial hydrogen mass fraction be $Y_0 = 0.007$ within the cloud, corresponding to a volume fraction of about 9%. The situation described by the equation 20 is expected, where viscous forces are negligible with respect to inertia forces. In fact:

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \ll 1 \qquad \Longrightarrow \qquad V = \sqrt{\epsilon g L} = 0.3\text{m/s} \tag{30}$$

and $\mathcal{D} \ll L\sqrt{\epsilon g L} = 0.03\text{m}^2/\text{s}$.

This means that the driving time scale is $\tau = \tau_c = 0.3\text{s}$. The hydrogen cloud rises up as a bubble. The flow can be reasonably considered as inviscid and the light gas is mainly transported by advection, since it is $\text{Pe} = 4 \cdot 10^2$.

3.2 Hydrogen dispersion at a larger scale

Now, the same scenario is studied at the larger scale $L = 1\text{m}$. If the same $Y_0 = 0.007$ is used, the resulting velocity scale is a few higher. Nevertheless, the same phenomenology can be expected. In fact

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \ll 1 \qquad \Longrightarrow \qquad V = \sqrt{\epsilon g L} = 0.9\text{m/s} \tag{31}$$

The time scale is $\tau = \tau_c = 1$s and $\mathcal{D} \ll L\sqrt{\epsilon g L} = 0.9\text{m}^2/\text{s}$. As the Péclet number is $\sim 10^4$, the advective transport of hydrogen is even more considerable than in the previous case.

3.3 Helium dispersion at larger scale

What happens when the same experiment is repeated with helium? If the size and the volume fraction of the cloud are the same, the length is conserved, but the buoyancy is scaled. The choice to conserve the species volume fraction in the floating cloud is justified by the aim to easily recover critical concentrations (i.e. for studies on flammability). Therefore, the helium mass fraction is $Y_0 = 0.013$. Also the velocity and the time scale are conserved. In fact:

$$\frac{\nu_\infty}{L\sqrt{\epsilon g L}} \ll 1 \qquad \Longrightarrow \qquad V = \sqrt{\epsilon g L} = 0.9\text{m/s} \tag{32}$$

and $\tau = \tau_c = 1$s. Besides, $\mathcal{D} \ll L\sqrt{\epsilon g L} = 0.9\text{m}^2/\text{s}$ with the corresponding Péclet number of $\sim 10^4$. Therefore, the same conditions are reproduced than in the case of hydrogen.

As in the three cases the cloud follows the same behavior that has been described in section 2.2.1, the continuity equation degenerates in the form of the equation 15. Besides the Richardson number is equal to one and the Froude number is equal to 0.3.

4 Discussion and conclusions

The previous sections concerned the influence of length and buoyancy scaling on the flow dynamics of a buoyant cloud. For the selected parameters, the main features are conserved in the treated cases.

In the examples 3.2 and 3.3, helium behaves as an appropriate substitute for hydrogen: for the same Ri, the velocity scale is the same, as well as the time scale and the species transport mechanism. As long as the cause of the flow is of the same entity, and the reactions and the effects are driven by parameters of the same order, according to the governing equations there is no reason to get different flow regimes when the chemical species changes.

In other situations, a corresponding analysis should be performed. Likewise we did, it should start from the governing equations and focus on one case or one class [3, 15].

Anyway, in the planning of an experiment, together with the clear settling of the goals, the scaling bias should be taken into account in order to identify the conserved quantities and the scaled ones.

Experimental activity plays a major role in fluid-dynamics and thermal-hydraulics research. In the past, scaling methodologies have been the basis for the development of the aerospace and nuclear industry. Experimental activity is still essential to investigate physical phenomena, to perform safety analysis and to validate computational tools [16]. Performing scaled experiments may lead – whereas necessary – to save time and resources, may enable the separation of phenomena and the resolution of physical quantities.

Nevertheless, it is clear that the study of a situation at different scales may require more experiments than one at a 1:1 scale.

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