MIXING OF DENSE OR LIGHT GASES WITH TURBULENT AIR: A FAST-RUNNING MODEL FOR LUMPED PARAMETER CODES

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ABSTRACT

The release of gases heavier than air like propane, at ground level, or lighter than air like hydrogen, close to a ceiling, can both lead to fire and explosion hazards that must be carefully considered in safety analyses. Even if the simulation of accident scenarios in complex installations and long transients often appears feasible only using lumped parameter computer codes, the phenomenon of denser or lighter gas dispersion is not implicitly accounted by these kind of tools.

In the aim to set up an ad hoc model to be used in the computer code ECART, fluid-dynamic simulations by the commercial FLUENT 6.0 CFD code are used. The reference geometry is related to cavities having variable depth (2 to 4 m) inside long tunnels, filled with a gas heavier or lighter than air (propane or hydrogen). Three different geometrical configurations with a cavity width of 3, 6 and 9 m are considered, imposing different horizontal air stream velocities, ranging from 1 to 5 m/s.

A stably-stratified flow region is observed inside the cavity during gas shearing. In particular, it is found that the density gradient tends to inhibit turbulent mixing, thus reducing the dispersion rate.

The obtained data are correlated in terms of main dimensionless groups by means of a least squares method. In particular, the Sherwood number is correlated as a function of Reynolds, a density ratio modified Froude numbers and in terms of the geometrical parameter obtained as a ratio between the depth of the air-dense gas interface and the length of the cavity.

This correlation is implemented in the ECART code to add the possibility to simulate large installations during complex transients, lasting many hours, with reasonable computation time. An example of application to a typical case is presented.

1.0 INTRODUCTION

The simulation of fire behaviour, as well as the formation of toxic or explosive atmospheres under accident condition is often analysed with Computational Fluid Dynamics codes (CFD). These tools are obviously suitable for the detection of fluid motion field and mixing processes that can be responsible for heat and mass transfer, but are too heavy to run simulations of fire propagation through several rooms, corridors or tunnels, accounting for flame and smoke propagation, or the chemistry of combustion together with the thermodynamic response of atmosphere and structures.

In practice, lumped parameter computer codes represent a reasonable means for the engineering evaluation of accident scenarios in complex installations and long transients, which can provide proper boundary conditions (pressures, gas temperature and composition, flows, etc.) for further analyses of local condition and short transients with CFD tools.

In the aim to address this important issue in the framework of safety studies of electric power generation plants, CESI decided to extend the capabilities of its computer code ECART [1] to the field of risk studies involving fires and explosive atmospheres within power plants employing fossil fuels or electric transformers located in caverns.

The development of ECART was started by ENEL in the Eighties for nuclear power safety, mainly accounting for the propagation of radiotoxic substances, in line with the state-of-the-art of thermal-hydraulics, chemistry and aerosol physics [2-3]. This tool is not plant-dependent, and is capable to simulate the phenomena governing airborne transport and retention of dangerous substances throughout generic pipelines, plant components or rooms.

The ECART code construction and validation was widely supported by a pool of specialists in the field, mainly from University of Pisa and Politecnico di Milano. Further resources for its development came from European Union research programs, as well as from EDF and ENEA through ad-hoc agreements focused on nuclear safety research and applications. ECART development and maintenance are presently managed by CESI, market leader in testing and certification of electromechanical equipment and power system studies, that acquired ENEL's R&D department.

Whilst the code has been exhaustively tested and updated in the framework of several benchmarks against experimental data and through direct applications to nuclear power plants [4], the code modelling capabilities have been now extended to fire transients. This extension was carried out by CESI in the framework of the "electricity system research", Projects SISIGEN and SISET, whose funding has been provided by means of a levy on the electricity bills paid by the customers of the electric service. The modelling and analysis work is managed through scientific cooperations with the specialists of the Politecnico di Milano, the Politecnico di Torino and the University of Pisa [5-8].

The phenomena related to the dispersion of denser or lighter stratified gases, which are of considerable importance in the analysis of accident scenarios involving industrial plants containing flammable gases were recently addressed in the frame of a cooperation between the University of Pisa and CESI, having the purpose to upgrade the models implemented in the thermal-hydraulic model of the code for application in to fires and explosions. The work, in addition to perform a general review of the code models, introduced new modelling capabilities, including the simulation of turbulent diffusion of stratified gas from cavities in the ground or in the ceiling of tunnels. The main target of the introduction of the model is to provide ECART with reasonable predictive capabilities in relation to these phenomena when considering gases like propane, butane or hydrogen.

The model was developed on the basis of several calculations carried out by the fluid-dynamic code FLUENT [9], performed considering different geometries of the cavity included in a two-dimensional tunnel in which air flow is forced. The data concerning the turbulent diffusion mass transfer from the cavity to the tunnel obtained by the fluid-dynamic computer code were correlated in dimensionless form, considering the particular way in which the code simulates cross stream diffusion.

The implementation of the model in ECART was then validated predicting the same data adopted for devising its relationships, thus confirming the adequacy of the assumptions made in data regression. Finally, ECART was applied to a variable tunnel velocity transient, predicted also by the FLUENT code, in order to assess its adequacy in more general conditions.

2.0 MAIN FEATURES OF THE ECART CODE

ECART architecture is presented in Figure 1, where the dark boxes are the previously existing modules and the light boxes represent two recently developed modules. As can be seen, the code consists of three main sections, linked together by information transfer channels: a thermal-hydraulic section providing the boundary conditions, an aerosol-vapour section calculating the transport of radioactive or toxic substances through the analysed pathway and a section evaluating the chemical equilibrium among airborne compounds and some reaction kinetics between gases and solid materials.

The two specific modules added in recent work allow the analysis of fires accounting for pyrolysis and heat radiative transfer. Table 1 summarises the links between the modules as shown in Figure 1.

As ECART was set up to treat transport phenomena (mass, energy, momentum transfer and physicochemical processes) through generic flow systems with an Eulerian approach, it requires to subdivide the analysed domain into control volumes connected by flow junctions. The junctions are in turn subdivided into "explicit" and "implicit" junctions, according to the particular pressure-to-flow coupling adopted to evaluate fluid transport across them. Within each volume, it can simulate two-phase flow (air-mist) under conditions of vertical stratifications between the pool and the atmosphere (Figure 2), with possible formation/fallout of suspended water drops, while the gas phase is treated as perfectly mixed. The interaction between the fluid and the walls, as well as the heat conduction within the wall materials is also accounted for. The aerosol transport mechanisms (agglomeration, removal or resuspension) are accounted by models capable of describing the dependencies on particle size, shape and physic-chemical properties of gases and vapours.

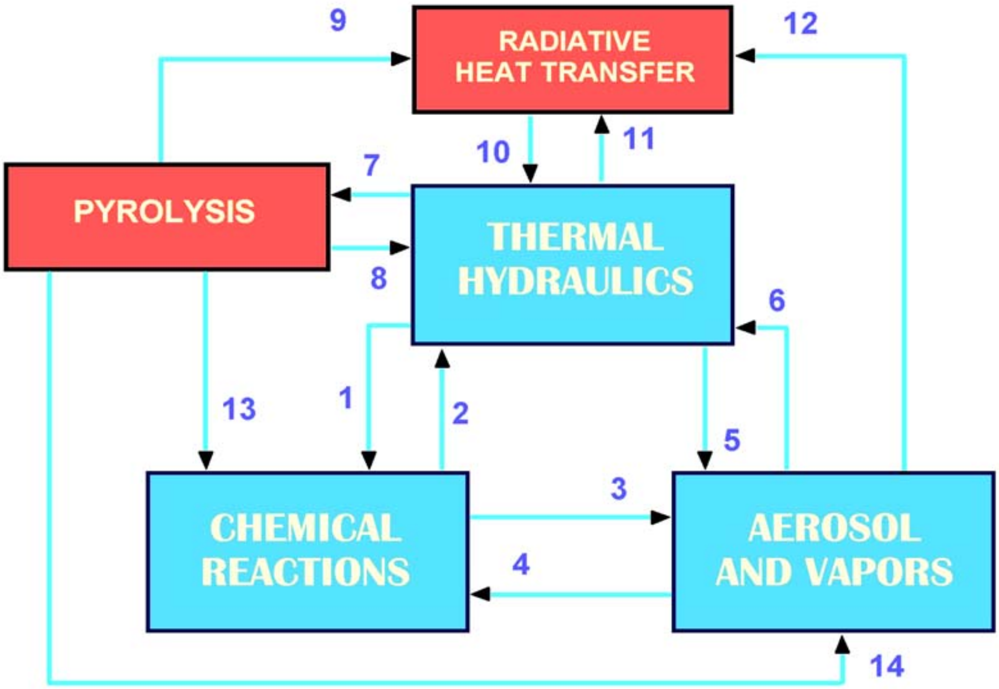


Figure 1. Scheme of the links among the main sections of the ECART code

Table 1. Links between the ECART modules

1. thermal-hydraulic boundary conditions for chemistry	7. heat fluxes to burnable structures
2. heat sources due to chemical reactions	8. temperature profiles of pyrolysing structures
3. update of composition of airborne phase	9. emissivities of pyrolysed surfaces
4. reactants concentration in gaseous phase	10. absorption factors for radiative heat transfer
5. thermal-hydraulic boundary conditions for vapors and aerosols	11. geometric parameters of flames
6. radioactive decay heat and influence of aerosol on gas properties	12. aerosol radiative parameters
	13. volatile products from pyrolysis
	14. soot generation from pyrolysis

The thermodynamic modelling available in ECART allows evaluating the thermal behaviour of materials and components subjected to damage and the effects of safety systems intervention, including also water injections, like sprinklers or scrubbers.

A feasibility study for the use of ECART on non-nuclear risk installation problems was recently performed by CESI through cooperation with Politecnico di Torino and Politecnico di Milano, by carefully reviewing the bases of fire phenomenology and considering, as references, a full-scale fire experiment [9] and a real fire scenario occurred within long motorway tunnels [10]. The analyses were addressed, respectively, to evaluate the hazard of combustion products, the damage to structures and were aimed to point out the limitations and capabilities of ECART in treating this kind of problems.

In the absence of fire models in the traditional version of ECART, lumped parameter nodalizations and simple boundary conditions were assumed, while the fire was provisionally simulated by time-varying boundary conditions: combustion gas sources and air suctions were pre-calculated and were not affected by the air flow transients predicted by the code itself.

The first difficulty encountered was the lumped parameter approach of ECART, chosen to permit the coupling with long-running aerosol and chemistry models. This is not the case of smoke transport through almost one-dimensional pathways and with well-defined combustion conditions. However, in order to solve cases in which strong 3D effects are encountered, some compromises in the nodalization criteria of the component interested by the combustion needed to be considered. After some sensitivity tests, it was decided to use a minimum number of control volumes, still permitting to describe typical “two-zone” behaviour or, in any case, the main convective motions around the flame. This simplified flow field can be tuned by adjusting the volume junctions parameters and fitting the available information on fluid-dynamic behaviour of the analysed scenario [11].

Anyway, the most important outcome of this feasibility study was a positive conclusion about the proposed target of extending ECART capabilities to fires, pointing out that the most significant open issues were just represented by the lack of a proper combustion model to simulate the behaviour of burning materials and the availability of air and the need to include the radiative heat transfer to the thermal-hydraulic section.

These models have been recently introduced in order to compensate for these lacks [12].

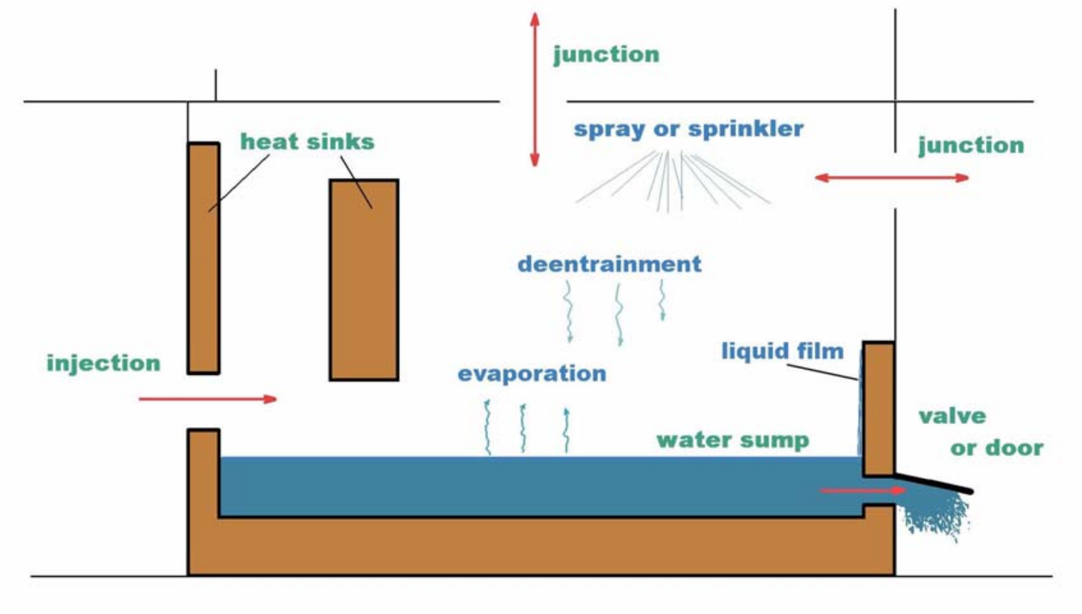


Figure 2. Control volume model adopted by the ECART thermal-hydraulics module

3.0 CFD ANALYSIS OF STRATIFIED GAS BEHAVIOUR

One of the geometrical conditions considered in the analysis of stratified gas behaviour in the presence of a shearing stream is reported in Figure 3. It consists of a two-dimensional tunnel in which an air flow is forced at the inlet and a pressure boundary condition is imposed at the outlet. The inlet part of the tunnel is 20 m long and it is separated by the 10 m long outlet part by a region in which a cavity is located. In preliminary calculations the cavity had different depth (2 to 4 m) while in the latest calculations performed in model development a single depth of 4 m was considered, as depth only affects the last part of the transients when the gas is almost completely removed. The considered lengths of the cavity were 3, 6 and 9 m.

The cavity is initially filled with gas mixtures heavier or lighter than air, considered as the shearing gas. In the case of gases heavier than air (propane and butane) gravity is downward directed, while with lighter gases (hydrogen) it is directed upwards; in this way, the same model can be used to simulate cavities in the ground or in a ceiling in which a flammable gas is initially stratified and is slowly removed by the action of the shearing stream; of course this implies the conservative assumptions that such a stratification has been possible, e.g. as a consequence of a direct injection of gas in the cavity.

The cavity region is discretised with great detail (cells with $\Delta x = 0.1$ m and $\Delta y = 0.05$ m) to avoid as far as possible numerical effects in the evaluation of the gas removal rates (Figure 4). The total number of cells for the whole domain depends from the geometrical configuration but it is about 8000 cells for the shortest domain.

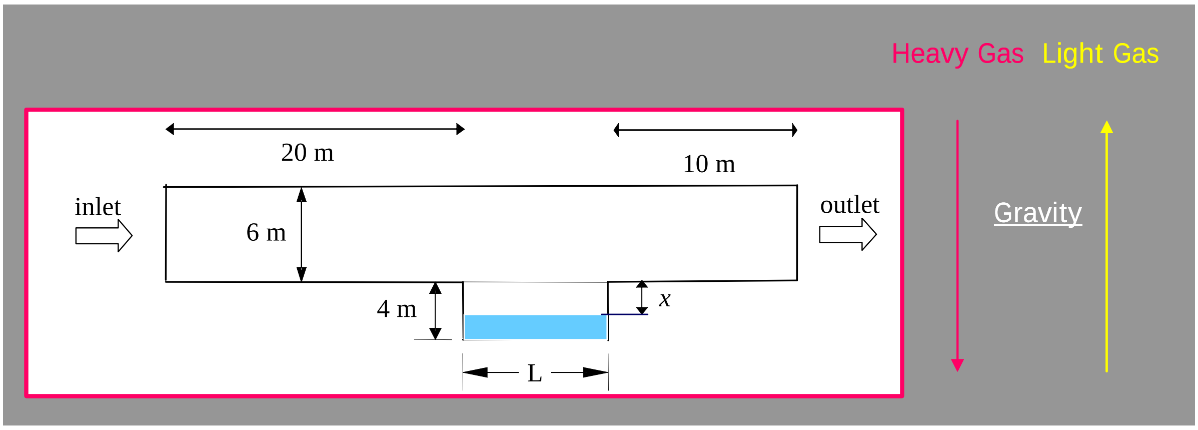


Figure 3. Computational domain adopted in the CFD calculations

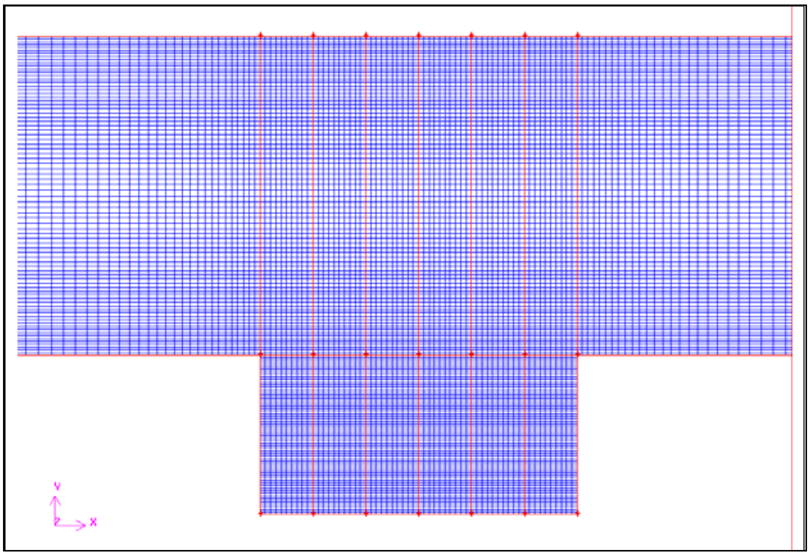


Figure 4. Detail of the spatial discretisation for the tunnel in the region of the cavity

On the basis of the experience gained in previous preliminary analyses, five different values of the average velocity of air in the tunnel were considered (from 1 to 5 m/s). Air enters the tunnel at a temperature of 300 K with uniform velocity distribution along the tunnel height. The adopted turbulence model is the standard κ-ε available in the FLUENT code, assuming an inlet turbulence intensity of 2%. This value is assumed as a reasonable parameter estimate, though sensitivity studies showed a negligible importance of inlet turbulence on the obtained results.

For the sake of collecting data on the effect of different parameters, the calculation is initialised to an ideal stratified situation by filling the cavity with the gas; the contact with the air stream is initially avoided by a wall which is suddenly removed at the start of the transient, initiating the de-stratification process. The code is made printing in separate files the values of the residual mass of gas in the cavity as a function of time, in order to let subsequent processing of the relevant data in terms of mean gas mass fraction.

Figure 5 reports two typical gas concentration distributions within the cavity during the de-stratification process. The two cases refer to propane gas and show a typical behaviour in which the gas behaves much like a liquid in a pool being progressively removed by the shearing stream. In such conditions the removal rate is continuous and amenable to be correlated on the basis of usual power law functions of classical dimensionless parameters, as it will be shown later on. However, the situation is not always simple; in some conditions the surface separating the stratified gas by the shearing stream becomes wavy, possibly due to the

inception of a Kelvin-Helmoltz instability. In such cases, the removal rate may increase considerably showing that the mechanisms for gas removal drastically change.
At this stage, only computational data are available to judge about the realism of such a phenomenon. As numerical problems may also affect the observed behaviour at an extent that is presently impossible to ascertain (e.g., convergence and diffusion), it was decided to discard the cases with wavy behaviour from the database for the development of the correlation. So, the validity of the obtained law must be considered limited to the cases of shearing with smooth surface.

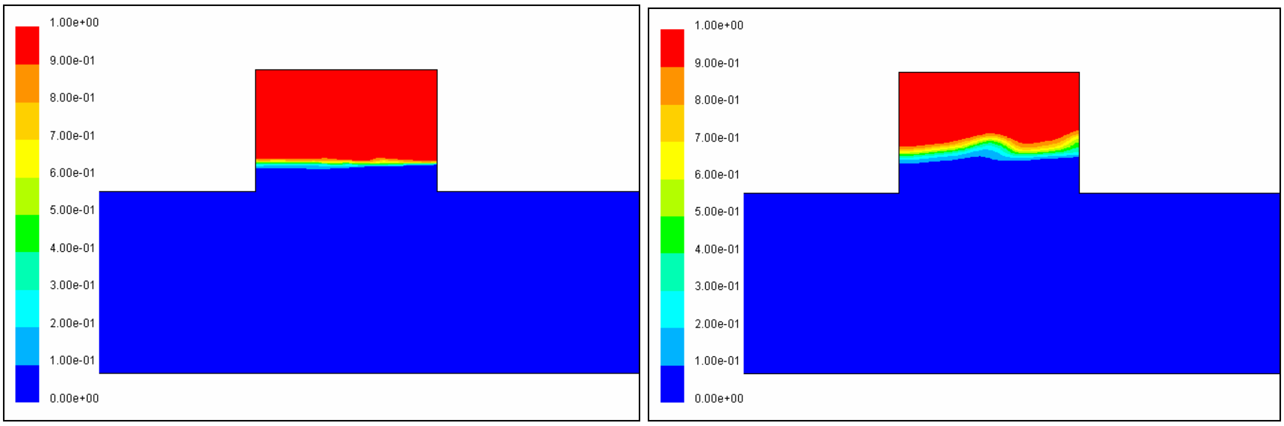


Figure 5. Typical concentration distributions during the de-stratification process of hydrogen with an air flow of 4 m/s (cavity 4 m depth and 6 m length)

4.0 MODEL DEVELOPMENT

With reference to Figure 6, the model for evaluating the de-stratification phenomenon due to turbulent diffusion developed for the ECART code assumes that the mixing effect is obtained as a result of two equal countercurrent mass flow rates, W_{diff}, occurring across the junction separating the cavity from the tunnel. This strategy was chosen also because the code already features a countercurrent flow model coming into play when a heavier fluid is located above a lighter one (as in Rayleigh-Taylor instability or flooding conditions); this pre-existing model, which can be considered a numerical artifact for avoiding unphysical density distributions across junctions, can be now adopted for dealing with the opposite case in which a stable density distribution is experienced, but the presence of shearing induces mixing.
As shown in Figure 6, whenever a countercurrent mass flow rate of gas is established between the tunnel and the cavity, the density difference of the two countercurrent streams gives rise to a net flow rate, W, needed to keep constant the number of moles in the cavity, as required by the constant pressure constraint. The presence of this net flow rate, which is positive (i.e., from the cavity to the tunnel) for an heavier gas and negative (i.e., from the tunnel to the cavity) for a lighter gas (note Figure 6 always shows the positive versus of this flow rate), must be accounted in both data fitting and in model implementation in the code.
On the basis of the constant mole constraint and considering that each flow rate transports a stream with the composition of the upstream volume, in the case of a heavier gas, it is

$$W_{diff} = \left(-\frac{dM_{hg,L}}{dt}\right)\frac{M_{hg} + \omega_{hg,L}\left(M_{air} - M_{hg}\right)}{M_{hg}\left(\omega_{hg,L} - \omega_{hg,U}\right)} \tag{1}$$

while for a lighter gas it is:

$$W_{diff} = \left(-\frac{dM_{lg,U}}{dt}\right)\frac{M_{lg} + \omega_{lg,L}\left(M_{air} - M_{lg}\right)}{M_{lg}\left(\omega_{lg,U} - \omega_{lg,L}\right)} \tag{2}$$

Therefore, on the basis of the computed time derivative of the stratified gas in the cavity it is possible to calculate the diffusion countercurrent flow rate to be assigned in the code. The assumption at the basis of the correlation is that the diffusion mass flow can be defined on the basis of a mass transfer coefficient by the following relationships:

$$h_{m,hg} = \left(-\frac{dM_{hg,L}}{dt} \right) \frac{M_{air}}{A_{cavity} M_{hg}} \qquad h_{m,lg} = \left(-\frac{dM_{lg,U}}{dt} \right) \frac{M_{air}}{A_{cavity} M_{lg}} \tag{3}$$

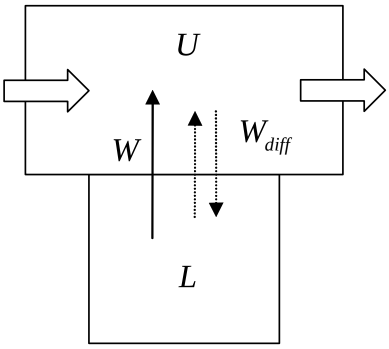
which hold respectively in the cases of the heavier and the lighter gas.
Considerations of the calculated data suggest that a correlation having the form:

$$St_{m,L} = \frac{h_m}{\rho_{air} \overline{w}_{air}} = \frac{Sh_L}{Re_L Sc} = x_1 \, Fr_x^{x_3} \left(x/L \right)^{x_4} \, R_\rho^{x_5} \tag{4}$$

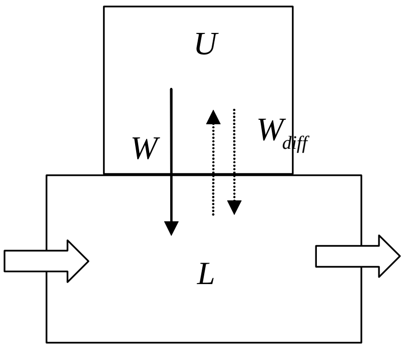
where it is

$$Sh_L = \frac{h_m L}{\rho_{air} D_g} \qquad Sc = \frac{\nu_g}{D_g} \qquad Re = \frac{\rho_{air} \overline{w}_{air} L}{\mu_{air}} \qquad Fr_x = \frac{\rho_{air} \overline{w}_{air}^2}{\left| \rho_g - \rho_{air} \right| g x} \qquad AR = \frac{x}{L} \qquad R_\rho = \frac{\rho_{air}}{\rho_g} = \frac{M_{air}}{M_g} \tag{5}$$

in which h_m holds for $h_{m,hg}$ or $h_{m,lg}$ in the cases of the heavier and the lighter gases respectively.
Least square optimisation of Eq. (4) over the set of data computed by the CFD code provide the coefficients of the correlation, that has been finally implemented in the ECART code.



a) heavy gas

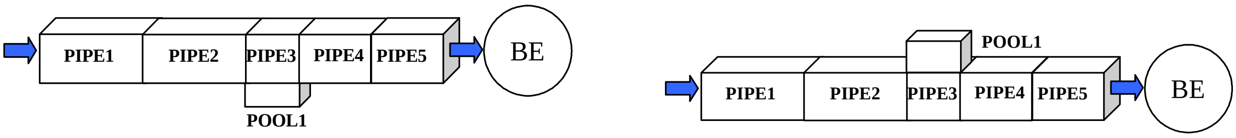


b) light gas

Figure 6. Scheme of the de-stratification model as implemented in the ECART code

5.0 COMPARISON BETWEEN ECART AND CFD CODE PREDICTIONS

In the aim to check the correct implementation of the model in the ECART code, the results of its application to the same calculation cases performed with the CFD code were analysed. The nodalizations adopted for the cases of propane and butane (heavier than air) and hydrogen (lighter than air) are shown in Figure 7 a) and b) respectively. The tunnel has been represented by 5 control volumes having square cross section (with a side of 6 m), while the cavity has been represented by a single volume, initially filled by the stratified gas. An air flow is forced inside the tunnel, while at the end of it a back environment provides to impose the required pressure constraint.
Figures from to 8 to 10 compare the results obtained by the ECART code with the data obtained by FLUENT for the average gas mass fraction in the cavity (named ANVOL-3 for ECART). As it can be noted the match between the curves is very close, showing that the assumptions adopted in developing the correlation and implementing the model in the ECART code are satisfactory. The steeper decrease in hydrogen mass fraction, with respect to the cases of propane and butane, is due to the greater difference between the molecular weights of hydrogen and air.
In order to compare the results of ECART with those of the CFD code in a case having greater relevance for code validation, a transient in which the air flow in the tunnel is made to vary from 0 to 3 m/s is considered. The cavity initially contains propane gas, in stratified conditions. Such a case is more representative of the cases to be addressed by the ECART code, since it involve a transient evolution of the shearing velocity as it is, e.g., during postulated incidents inside tunnels or other ventilated systems. The addressed cavity has a depth of 3 m and a length of 6 m.



a) heavier gas b) lighter gas

Figure 7. Nodalizations adopted for ECART

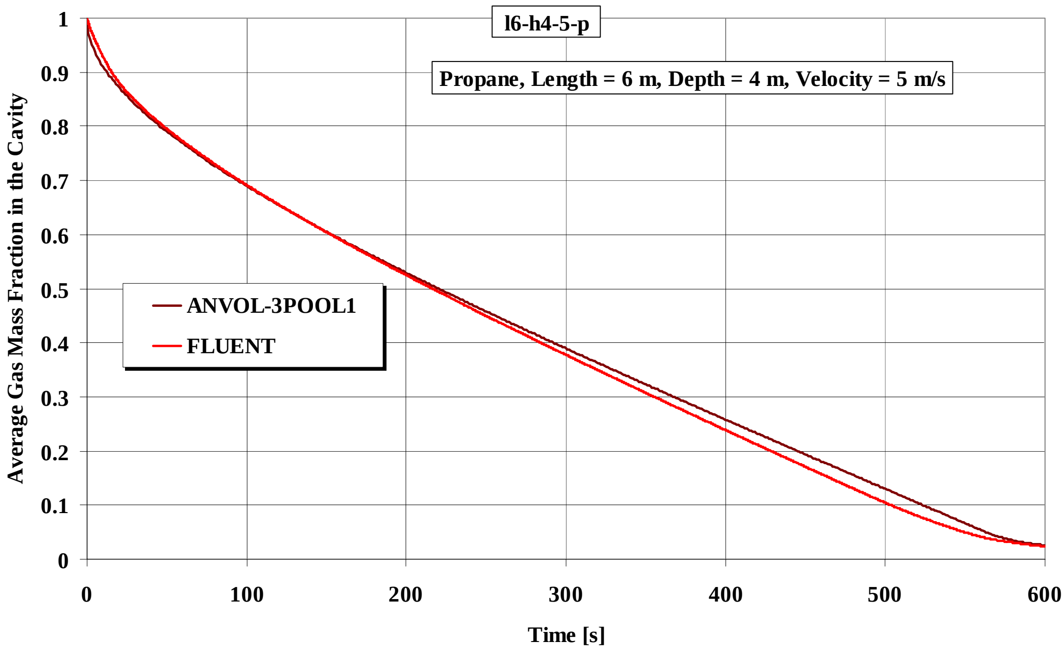


Figure 8. Comparison between ECART and FLUENT predictions for a case with propane

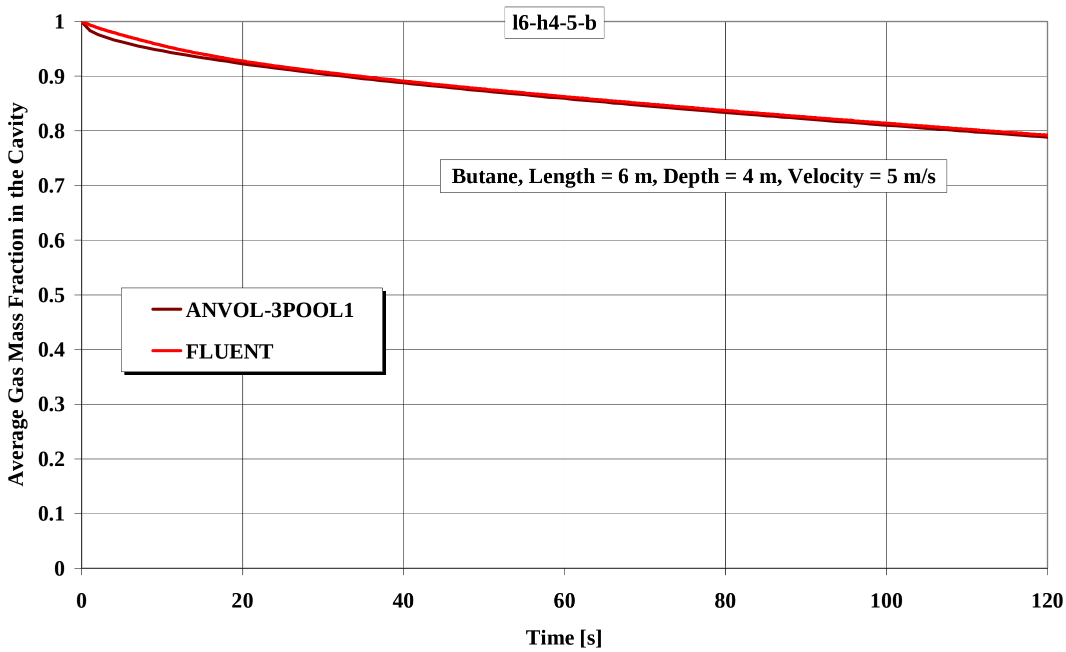


Figure 9. Comparison between ECART and FLUENT predictions for a case with butane

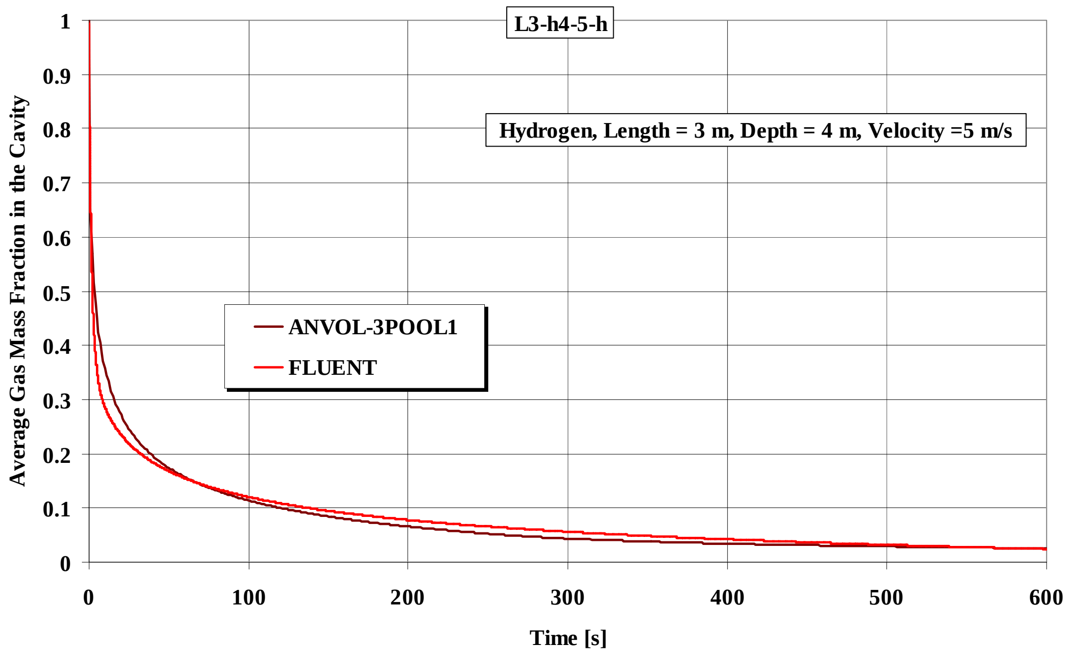


Figure 10. Comparison between ECART and FLUENT predictions for a case with hydrogen

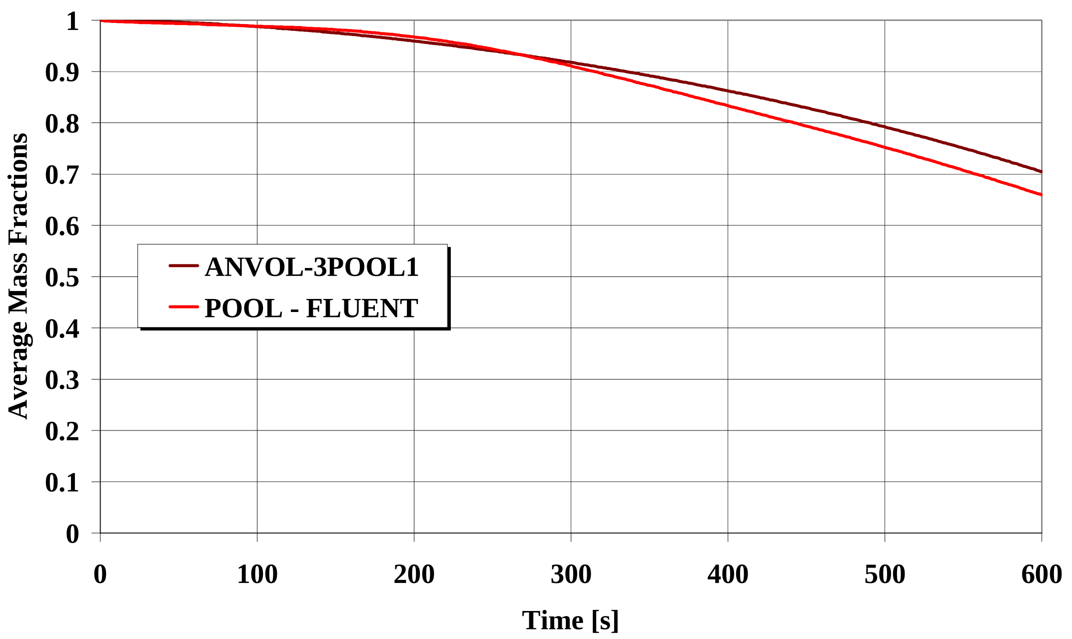


Figure 11. Comparison between ECART and FLUENT predictions for a case with propane and air velocity increasing from 0 to 3 m/s in 600 s

Figure 11 compares the results obtained by ECART and FLUENT in terms of average gas mass fraction in the cavity. A reasonable match between the data provided by the two codes appears, thus confirming the coherence of the two numerical models. The advantage of ECART in term of fast running capabilities more than compensates for any possible observed inaccuracy.

6.0 CONCLUSIONS AND FUTURE PERSPECTIVES

The model included in the ECART code for simulating de-stratification of stratified gases in cavities by shearing flows shows a satisfactory behaviour in comparison with CFD code predictions. At this regard the following considerations apply.

- The model has been devised on the basis of calculated data instead of experimental ones. This procedure relies on the capability of the CFD code to correctly represent the addressed phenomena, which cannot be anyway given for granted. In science, as well as in engineering, the only decisive aspect is obviously experience; so, the model cannot be considered really validated unless a convincing comparison with experimental data is provided.
- On the other hand, experimental data applicable to the considered situation cannot be easily found. In this respect, the adoption of a CFD code for setting up a physical correlation provides guidance in proposing the general features of a constitutive law. It is well known, that detailed numerical codes can be considered suitable in this aim; however, any model devised in such a way cannot be better than the code from which data have been obtained for its validation.
- In this case, the worth of the work performed is to get in a fast running way predictions similar to the ones that could be obtained by lengthy CFD calculations for a particular phenomenon, being in our case the de-stratification of a gas from a cavity due to a shearing gas stream.
- Of course, limitations apply to the model. In addition to the already mentioned exclusion of oscillatory surface phenomena, it must be mentioned that no allowance was here made for 3D effects, like a finite extension of the cavity in the third coordinate.

These observations ask for future work on this subject that should be aimed at collecting experimental data, either from the available literature or produced by original experiments. This represents the task to be completed to gain further insight into the fascinating phenomena shown by such a simple but technically relevant issue.

NOMENCLATURE

Roman Letters

A_{cavity}	area of the cavity [m^2]
AR	"Aspect Ratio"
D	diffusion coefficient [m^2/s]
Fr_x	Froude modified number
g	gravity [m/s^2]
h_m	mass transfer coefficient [kg/(m^{2}s)]
H	cavity depth [m]
L	cavity length [m]
M	mass [kg]
M	molecular weight [kg/mole]
n	mole number [mole]
Re	Reynolds number
Sc	Schmidt number
Sh_L	Sherwood number
St_m	mass transfer Stanton number
t	time [s]
w	velocity [m/s]
W	mass flow rate [kg/s]
x	depth of gas surface in the cavity [m]

Greek Letters

μ	dynamic viscosity [kg/(ms)]
ν	kinematic viscosity [m^2/s]
ρ	density [kg/m^3]
ω	mass fraction

Subscripts

air	air
cavity	cavity
diff	turbulent diffusion
g	referred to the generic stratified gas or
hg	heavy gas
lg	light gas
L	lower volume
U	upper volume

Superscripts

$\overline{\circ}$	average value

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