ADVANCES IN THE DEVELOPMENT OF A FLUID-TO-FLUID SIMILARITY THEORY FOR FLUIDS AT SUPERCRITICAL PRESSURE: RESULTS FROM SENSITIVITY ANALYSES

A. De Angelis, A. Pucciarelli*, S. Kassem, W. Ambrosini
Dipartimento di Ingegneria Civile e Industriale, Università di Pisa, Italy
*Corresponding Author: andrea.pucciarelli@dici.unipi.it

ABSTRACT

In the present paper, the capabilities of a similarity theory for heat transfer to supercritical pressure fluids are further investigated with respect to past work, widening the range of the addressed operating conditions. In particular, experimental data for water at 25 MPa are here considered; several cases addressed adopting different simulant fluids (i.e. CO_2, NH_3 and R23), in order to understand possible dependencies of the proposed rationale on the imposed mass flux and the observed heat transfer conditions. The obtained results confirmed the lessons learned from the recent analyses, though highlighting some possible needs for improvements in both the adopted CFD model and the similarity rationale in some specific operating regions.

The aim of the present paper is to show further results in relation to the capabilities of the proposed theory, which seems sufficiently mature to be now considered for validation against experimental data.

Keywords: SCWR, supercritical fluids, heat transfer, similarity

NOMENCLATURE

Roman Letters

C_p	specific heat at constant pressure [J/(kg K)]
D	diameter [m]
Fr	Froude number [-]
g	gravity [m/s^2]
G	mass flux [kg/(m^{2}s)]
Gr	Grashof number [-]
h	specific enthalpy [J/kg]
k	thermal conductivity [W/(m K)]
L	length [m]
N_{SPC}	sub-pseudocritical number [-]
N_{TPC}	trans-pseudocritical number [-]
Nu	Nusselt number [-]
Pr	Prandtl number [-]
q''	heat flux [W/m^2]
$\dot{Q}$	power [W]
Re	Reynolds number [-]
Ri	Richardson number [-]
St	Stanton number [-]
T	temperature [°C]
w	velocity [m/s]
W	mass flow rate [kg/s]

Greek Letters

β	isothermal expansion coefficient [K]
μ	dynamic viscosity [kg/(m s)]
ν	kinematic viscosity [m^2/s]
ρ	density [kg/m^3]

Superscripts

*	dimensionless value
$\overline{\circ}$	(overbar) average value

Subscripts

b	bulk value
D	based on diameter as length scale
DB	based on Dittus-Boelter correlation
$fluid-i$	related to the i-th fluid
in	inlet
loc	local
out	outlet
pc	pseudocritical

w wall value

ρ based on density for buoyancy effects

1. INTRODUCTION

In order to improve the competitiveness of nuclear power plants with respect to other advanced power generation processes, such as gas-coal combined-cycles and supercritical coal-fired power plants [1], and to achieve a better utilization of the nuclear fuel, in 2002 six Generation IV concepts of nuclear reactors were proposed in the frame of the Generation IV International Forum (GIF). Those concepts, as reported by the forum itself, *"[…] will use fuel more efficiently, reduce waste production, be economically competitive, and meet stringent standards of safety and proliferation resistance"* (from the GIF portal). Gen IV concepts would lead to a higher efficiency of the power plants (e.g., around 45% to 48%, see [2]), increased simplicity in the plant layout, improved safety and decrease of the energy specific costs.

Among the six Generation IV concepts, the Super Critical Water-cooled Reactor (SCWR) uses supercritical light water as coolant and operating fluid. During the years, several concepts of SCWR have been presented by different countries that have supported this project, mostly referred to modern PWRs using a Pressure Vessel type reactor. The value of coolant pressure is in the range of 25 MPa (see e.g., [2]), while different layout choices are considered, such as the number of loops of the thermodynamic cycle, the type of neutron spectrum and more. A different concept was proposed by the Atomic Energy of Canada Limited (AECL), now NCL, which takes its main characteristics from the present CANDU reactors, being pressurized channel type ones, and are moderated with heavy water while cooled with supercritical light water.

However, even if some conceptual design has been already developed, mainly based on LWR reactor technology, some critical issues are still present, making difficult the practical achievement of the first SCWR prototypes. These issues cover chemical problems about supercritical water radiolysis, material issues (as corrosion) and thermal-hydraulic ones. In particular, there is a need for a large heat transfer to fluids at supercritical pressures, in order to validate the models able to simulate normal operating conditions and postulated accidents in the future SCWR: better knowledge and predictive capabilities of the involved heat transfer regimes could be desired. In experimental activities, the use of water in prototypical conditions is obviously the best option, though sometimes the adoption of simulant fluids can be preferable for their less demanding conditions in terms of design parameters and for higher safety in operation during the experiments.

Carbon dioxide and refrigerant fluids are often used in experimental facilities, trusting in a similar behavior with respect to water. In designing such experiments, similarity in heat transfer between the model fluid and supercritical water needs to be established, requesting a sufficiently well assessed rationale. This rationale is also useful in general terms, because it is based on the consideration of the most relevant dimensionless numbers for heat transfer phenomena: this allows clarifying the way in which correlations and other heat transfer predictive tools should be formulated to hope to be successful enough.

In the past years, several studies were performed in order to propose similarity theories for heat transfer to supercritical pressure fluids by performing studies of the involved phenomena (see e.g., [3-5]). These studies sometimes obtained reasonable results, even if in a strict range of conditions not too close to the pseudocritical threshold or not involving deteriorated heat transfer, where the deviations start to become important [6]. However, the intrinsic complexity of the phenomena made some authors to reach the sad conclusion that a complete and reliable theory in this regard is very difficult to achieve.

In this work, further information on a recently proposed similarity theory, developed on a theoretical basis with supporting RANS calculations, are presented (see [7-9]). This further work was obtained during a MSc thesis work performed at University of Pisa [10]. In this work, experimental data by Watts [11] are considered, while three model fluids are adopted, as in previous works: carbon dioxide, refrigerant R23 and ammonia. The first two fluids were chosen for their previous adoption in experimental facilities, also due to their more manageable critical conditions, while ammonia is considered in the analyses just for its closer thermal behavior with respect to water (see [12]), though it could be not advisable to be really used in experiments.

In the mentioned recent work [10], after further validation of the adopted CFD model against the considered water experimental data [11], the similarity is applied to the best-predicted data set. This was the same adopted in previous studies (see e.g., [13]-[15], [8]) to support the assessment of the similarity theory.

Another reference work that is taken into account in this paper is a very recent one [9], which used the similarity rationale here in discussion to address experimental data obtained with carbon dioxide by Kline [16], showing excellent data in reproducing similar trends for the same fluids addressed here. It can be anticipated that the results obtained in the present case are less exciting than those obtained in [9], thus providing both confirmations and warnings about the applicability of the similarity theory on the basis of information available by the adopted CFD model.

2. ADOPTED SIMILARITY THEORY

2.1 The rationale

The theoretical bases of the adopted similarity theory were set in the work by Pucciarelli and Ambrosini in 2016 [13], adapting and better discussing dimensionless parameters proposed in a paper on flow stability in heated channels with supercritical pressure fluids [17], on the basis of suggestions coming from the field of two phase flow. The similarity theory, after providing promising results supported by DNS [18], was then applied in a local form [7] and then generalized to a form applicable to a broader range of boundary conditions [8]. Kassem et al. [9] provided a further assessment of the theory on the basis of the application to carbon dioxide data [16]. While referring the reader to the above mentioned papers for a more detailed discussion, some of the principles of the theory are summarized herein.

The key observation in this frame is that a good representation of heat transfer phenomena with supercritical pressure fluids has a critical dependence on the prediction of the fluid density distribution along and across the flow duct. This is proven by the fact that phenomena like heat transfer enhancement and deterioration are tightly linked to the lightening of the fluid close to the wall and along the duct: in fact, heat transfer enhancement and deterioration depend or are simultaneous to the strong changes in fluid density close to the pseudocritical threshold. In fact, heat transfer enhancement mostly occurs close to the pseudocritical temperature, where the density experiences a considerable drop, and deterioration is determined by both buoyancy and acceleration phenomena, again due to the changes in density, mostly at the pseudo-critical threshold and across it.

A strong link exists between fluid density and specific enthalpy when evaluated in the dimensionless forms $\rho^* = \rho / \rho_{pc}$ and $h^* = \left(h - h_{pc}\right) \beta_{pc} / C_{p,pc}$, representing a nearly unique trend for the different fluids considered herein and for a large range of supercritical pressures. On this basis, "similar" conditions are defined as those which provide the same distributions of dimensionless specific enthalpy and hence of dimensionless density along and across the flow duct.

Some results, whose detailed explanation is reported in previous works [8, 13], are as follow:

- in order to achieve similar conditions, the bulk dimensionless inlet subcooling and the change in bulk specific enthalpy across the channel must be the same, something obtained by preserving $N_{SPC} = -h_{in}^* = -\left(h_{in} - h_{pc}\right) \beta_{pc} / C_{p,pc}$ and $N_{TPC} = \left(\dot{Q}/W\right) \beta_{pc} / C_{p,pc}$, which account for the dimensionless specific enthalpy and power-to-flow ratio; it must be noted that the preservation of these two dimensionless numbers assures a proper similarity in bulk density changes and then in bulk acceleration effects;
- to preserve buoyancy effects, it is also necessary to preserve the Froude number at the inlet, $Fr_{in} = w_{in}^2 / gD$, something that, combined with the equality of the trends of dimensionless specific enthalpy and density at the wall (implied by the above definition of "similarity") also assures the preservation of the Froude number and of the Richardson number, $Ri_D = \left[\left(\rho - \rho_w\right) gD\right] / \rho w^2 = Gr_{D,\rho} / Re_D^2$ all along the duct, as a very useful consequence;
- by also imposing the same Reynolds number at the inlet it is possible at least to try preserving turbulence scale effects, though it is not possible s to achieve this result all along the duct, owing to the unavoidable different changes in kinematic viscosity for different fluids due to heating; however, the simultaneous requirement of preservation of Froude and Reynolds numbers results in the need to change the pipe diameter and inlet velocity according to the formulations:

$$\frac{D_{fluid-2}}{D_{fluid-1}} = \left[\frac{\nu_{in,\,fluid-2}}{\nu_{in,\,fluid-1}}\right]^{2/3} \quad \text{and} \quad \frac{w_{in,\,fluid-2}}{w_{in,\,fluid-1}} = \left[\frac{\nu_{in,\,fluid-2}}{\nu_{in,\,fluid-1}}\right]^{1/3} \tag{1}$$

- the choice of pressure for the simulant fluid has been the subject of the proposal of different rationales; in place of preserving the reduced pressures, as in many previous theories, actually the attention was firstly given to the identification of "similar" pressures at which the Stanton numbers or the Prandtl numbers of the fluid could have similar trends along the channel, i.e., trends that can be scaled to each other as far as possible by constant factors (see the discussions in [13] and the more recent ones in [8] and [9]); it must be explicitly mentioned that this rationale is strictly depending on the trend of fluid properties in the flow duct and on our knowledge about them, configuring the hardest difficulty to be overcome in establishing the similarity rationale;
- the Stanton and the Prandtl numbers mentioned above are defined as $\overline{St} = Nu / Re\overline{Pr}$ and $\overline{Pr} = \overline{C}_p \mu / k$, where it is by definition $\overline{C}_p = \left(h_w - h\right) / \left(T_w - T\right)$; in this context, a useful form of the Newton's law of convection is the following:

$$N_{TPC} = \overline{St}\left(h_w^* - h^*\right) 4L/D \tag{2}$$

suggesting to compensate any discrepancy in the averaged Stanton number between the two fluids by changing the length over diameter ratio, while preserving the trans-pseudocritical number, making use of the formulation:

$$N_{TPC} = \left[q'' \beta_{pc} / GC_{p,pc}\right]\left(4L/D\right) = N_{TPC,loc}\left(4L/D\right) \tag{3}$$

this suggests that when changing the length over diameter ratio, iterations must be performed on the value of the heat flux to achieve the best "similarity", mostly monitoring the trends of the wall dimensionless specific enthalpy for the reference and the simulant fluids.

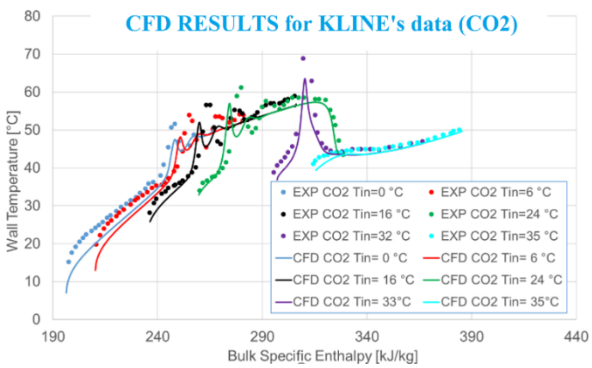
The above rationale, which may look somehow complex, is actually applied at present time in a rather systematic and straightforward way, following the steps described in the previous works ([13], [8] and [9]), with only the single challenging aspect that iterations on the heat flux must be done by CFD computations. In a future experimental application, while trying to reproduce a target wall temperature trend observed or assumed in a reference fluid with a model one, such iterations should be done also in the power supplied to the heated section, leaving sufficient flexibility in its heated length in order to change simultaneously the *L/D* ratio.

The strong incentive for the application of this similarity rationale is that, with some effort, it works, sometimes in an excellent way, and sometimes in a less exciting way, as it is for the results produced in this paper, which have the value to show merits and limitations of the present rationale.

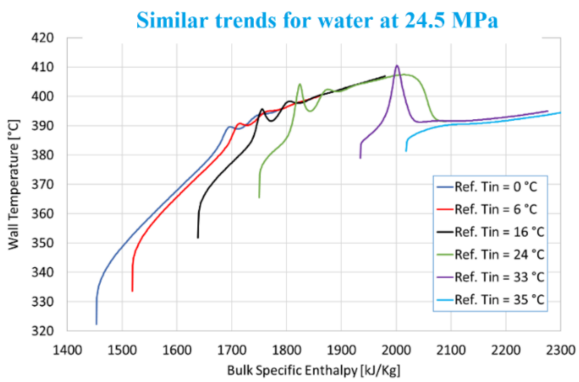
However, in the Authors' opinion, this rationale may represent a viable way for planning counterpart experiments, once its features and capabilities will be confirmed not only by RANS or DNS computations, as it was up to now, but also via ad hoc experiments.

2.2 Previous results and usefulness of the theory

One of the possibly most meaningful ways to show the usefulness of the similarity theory is presented in Figure 1, where the comparison with some of the addressed experimental data by Kline [16] and the CFD model predictions presented in [9] is firstly reported (Figure 1a). The data refer to the cases with CO_2 at 8.35 MPa, 4.6 mm ID, q"=20 kW/m^2, G=300 kg/m^{2}s, upward flow and different inlet temperatures.



a) original CO_2 experimental data prediction



b) prediction of similar water trends for wall temperature

Figure 1. Comparison of predictions for some Kline's CO_2 data with corresponding similar trends evaluated for water in similarity (adapted from [9])

As it can be noted, the experimental data, which are reasonably well represented by the CFD model, involve conditions with normal heat transfer, deteriorated heat transfer, at different levels, and final restoration of heat transfer at the transition to gas-like conditions (see e.g., [15] for an explanation of this phenomenon). This offers a full range of phenomena expected in SCWR operating conditions.

The strategy of using the similarity theory leading from Figure 1a to Figure 1b can be summarized as follows:

1. try reproducing with reasonable accuracy some target experimental data of interest: in fact, only if the CFD model is able to represent the observed phenomena with some fluid we may have some reliance on its correct representation of the same phenomena with some other, as a necessary though not sufficient condition to establish similar boundary conditions;
2. try obtaining similar results in terms of dimensionless specific enthalpy at the wall as a function of bulk enthalpy by applying the described similarity rationale;
3. when a reasonable match in terms of dimensionless specific enthalpy at the wall is obtained, the dimensionless trend can be translated into the dimensional one of water, obtaining temperature trends as shown in Figure 1b.

As it can be noted, the relevance of Figure 1b lies in showing how some trends obtained with a simulant fluid in Figure 1a can be translated to a postulated behavior of water, something that would justify the meaningfulness of the simulant fluid data whenever the target phenomena for water are really those depicted in Figure 1b. This is definitely a valuable information for assessing the usefulness of experimental data obtained for simulant fluids in view of the design at SCWR operating conditions.

3. CFD MODEL VALIDATION ON WATTS DATA

In some way, the process shown in the present work is reversed with respect to the one presented by Figure 1, since in this case we start from experimental data obtained with water and we try to argue how similar data could have been achieved by a simulant fluid. Again, the CFD model is the only relatively reliable means for obtaining this result. This inverse problem is perhaps the most important one when designing a facility with a simulant fluid, since the experimentalist could adjust the geometry, the power, the flows and other boundary conditions to achieve something representative of postulated relevant experimental conditions with water.

Indeed, Watts data [11] are already close to prototypical conditions, being obtained with water at 25 MPa and spanning over a range of flow and thermal parameters of interest for SCWR. Nevertheless, we now apply the similarity rationale to inquire if one or more of the selected simulant fluids could have been used to achieve the same information in dimensionless form. The advantage of such an procedure is obvious, considering that the critical parameters of the other fluids are less demanding in terms of high pressures and temperatures, thus decreasing the burden of safety requirements for the operation of an experimental facility.

Following the three steps described in the previous section, the first action to be done to apply the similarity rationale is to assure that the reference experimental data are reasonably well predicted by the CFD code. It is evident, in fact, that the lack of a proper assessment of the model in front of the exact data to be reproduced would discourage from making any similarity analysis based on computational means. In our case, the data by Watts are addressed to ascertain which of the experimental conditions can be reasonably reproduced.

The details of the adopted computational model have been described in previous mentioned works (see e.g., [13]) and are not repeated here, for the sake of brevity. It is just recalled that a 2D axial-symmetric discretization is adopted, with considerable refinements close to the walls in order to achieve a meshing compatible with the requirement of a wall y^+ much lower than unity, as requested by low-Reynolds number models. The specific model adopted is implemented in the STAR-CCM+ code [19] and is based on the standard low-Reynolds k-ε model available in the code [20], corrected by the introduction of an Algebraic Heat Flux Model (AHFM) devised during the PhD thesis of one of the authors [21]. Fluid properties are evaluated with the Refprop7 version of the NIST database [22].

Figure 2 to Figure 5 present the comparisons between experimental data by Watts [11] and the results of the CFD model. As an overall remark, the data are predicted rather correctly, considering the generally unsatisfactory state-of-the art in the field, though discrepancies do appear. In particular:

- for values of inlet temperature equal to 150 and 200 °C, the representation of heat transfer phenomena by the CFD code is generally correct, except for an intermediate value of mass flux, at which the CFD code predicts a milder deterioration; it must be noted that sensitivity analyses, made on purpose, showed that slight changes of mass flux or heat flux in the considered range considerably affect the response; this is a known characteristic of both experimental data and predictions of deteriorated heat transfer, linked to the great sensitivity of the onset of the phenomenon to details of the boundary conditions;
- with the exception of the above explained discrepancy, the quality of the obtained results is reasonable, up to a temperature of 250 °C; in the cases at 310 °C, predictions worsen, showing the tendency to overestimate deterioration as a sign that the model should be better tuned for these water conditions close to the pseudocritical threshold.

Once the model has been compared to experimental data, it is clear the level of reliability it can provide in the similarity analysis. Basing on this awareness, it possible to proceed further.

4. APPLICATION OF THE SIMILARITY THEORY

The set of experimental data chosen for the application of the theory was that referred to inlet temperature of supercritical pressure water of 250 °C and heat flux of 400 kW/m^2. This choice was made for a few main reasons:

- N_{SPC} is not too large for these data, thus avoiding reaching the freezing point of CO_2.
- the considered set of data was the best in terms of prediction by the CFD model
- moreover, part of this set of data was already considered in previous work [8], allowing to complete the analysis of a wider series of data;

For the sake of clarity, Figure 6 reports the CFD model predictions of the four mass flows belonging to the cases considered for the application of the similarity theory.

As it can be noted they involve trans-pseudocritical values of temperature. The four selected cases represent a set of experimental data at the same inlet temperature (i.e., same N_{SPC}) and heat flux, at different mass fluxes.

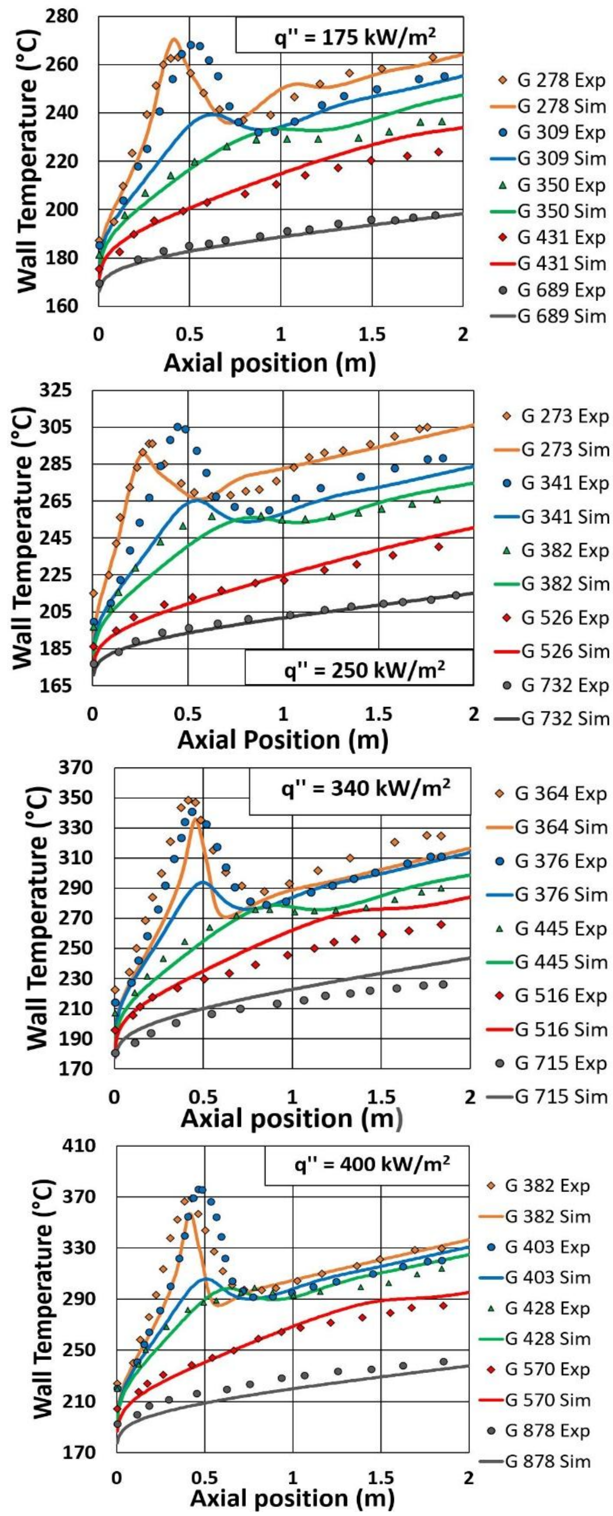


Figure 2. CFD results for Watts data at T_{in}=150 °C

As it can be noted, the increase in mass flux progressively decreases the level of heat transfer deterioration, up to the point in which a sort of normal heat transfer is obtained. These phenomena are predicted by the CFD code in a reasonable way, though quantitative discrepancies do appear.

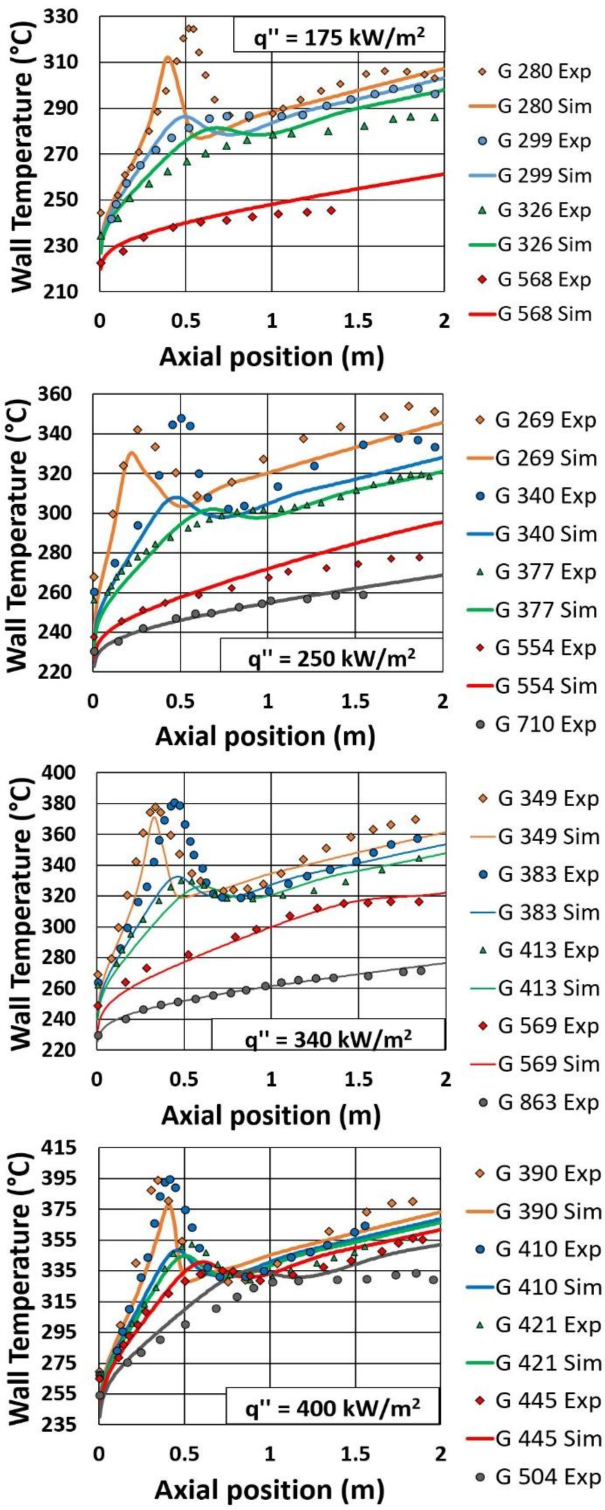


Figure 3. CFD results for Watts data at T_{in}=200 °C

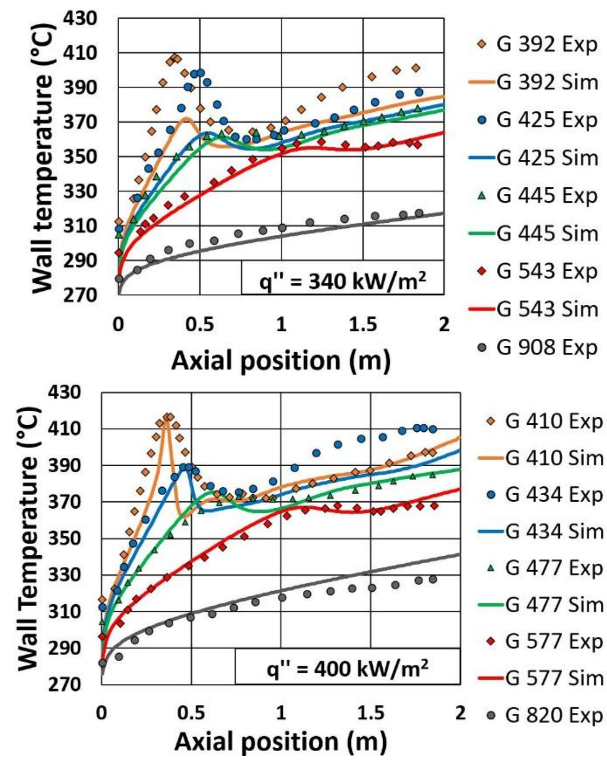


Figure 4. CFD results for Watts data at T_{in}=250 °C

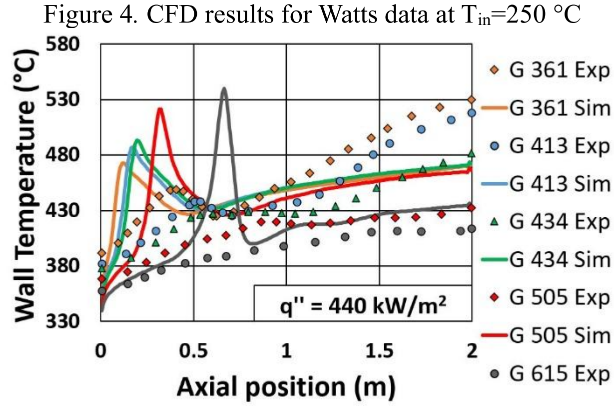


Figure 5. CFD results for Watts data at T_{in}=310 °C

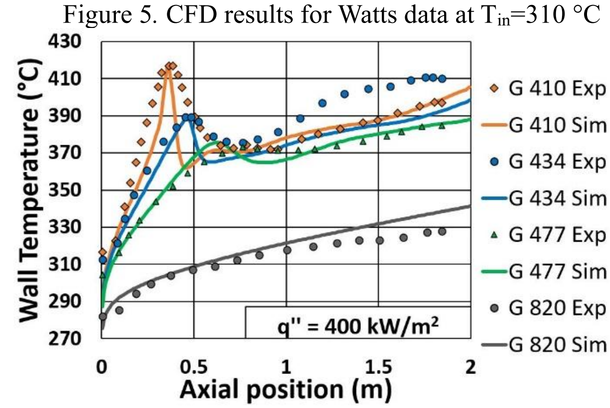


Figure 6. Selected CFD results for Watts data at T_{in}=250 °C and 400 kW/m²

Figure 7 to Figure 14 summarize in sequence the results obtained by the application of the similarity theory to the four described cases showing both correct and displeasing features.

In particular, Figure 7, Figure 9, Figure 11 and Figure 13 visualize the process of iteration on the heat flux to be performed in achieving the best possible match among the curves of dimensionless enthalpy at the wall as a function of dimensionless bulk enthalpy. On the other hand, Figure 8, Figure 10, Figure 12 and Figure 14 present the results obtained for the identified "best" values of heat flux.

Among the features correctly predicted for the four fluids, the early deterioration peak is represented with coherence with the reference water data for all fluids. This confirms the rationale at the basis of the similarity theory, at least concerning the occurrence of this early deterioration. The displeasing features are instead represented by oscillations in the dimensionless enthalpy at the wall observed for CO_2 and R23, especially in the cases with largest deterioration. These oscillations, to be interpreted as cycles of deterioration and recovery that are sometimes observed also in experimental data, do not appear in the reference water data nor in the predictions with NH_3.

A fully reliable explanation of these discrepancies is not available at the moment, since on one side we are using a CFD model having a limited accuracy and, on the other side, the four fluids have enough different properties. So, even considering the fact that the adopted model is approximate, it is not possible to exclude that what observed by calculations represents a real tendency to deterioration that could be found also in experiments with CO_2 and R23.

If real, this would break the almost perfect similarity achieved by the present theory in other cases (see e.g., [9]). A justification of this possible behavior could be traced to the difference in the fluid properties that, perhaps by chance for this particular operating conditions, combine to provide divergent behavior for fluids with higher Prandtl number (CO_2 and R23), with respect to fluids with lower values (water and ammonia).

Indeed a greater similarity between water and ammonia with respect to other fluids was already noted long ago [12].

In this regard, it is of little consolation the fact that, for lower degrees of deterioration, oscillations appear to be less and less important. However, this observation serves at least to diagnose that most of the observed oscillations occur across the transition through the pseudocritical threshold at the wall ($h_w^* = 0$), retrieving the dilemma, to be solved only by experiments, if these observed trends are an artifact of the CFD model or can be really observed.

Figure 15 illustrates the trends of the relevant dimensionless numbers along the channel. The level of similarity in the representation of the dimensionless wall enthalpy has an obvious effect on the Richardson number, on the ratio of the Nusselt number to the one obtained by the Dittus-Boelter correlation and on the product $\overline{St}(L/D)$. On the contrary, the Froude number, depending only on bulk variables, shows no effect of these discrepancies and exhibits a unique trend for all the fluids, as expected.It is finally mentioned that more many data than shown here were collected in this work, which are available in the MSc Thesis in whose frame it was performed, made available online [10].

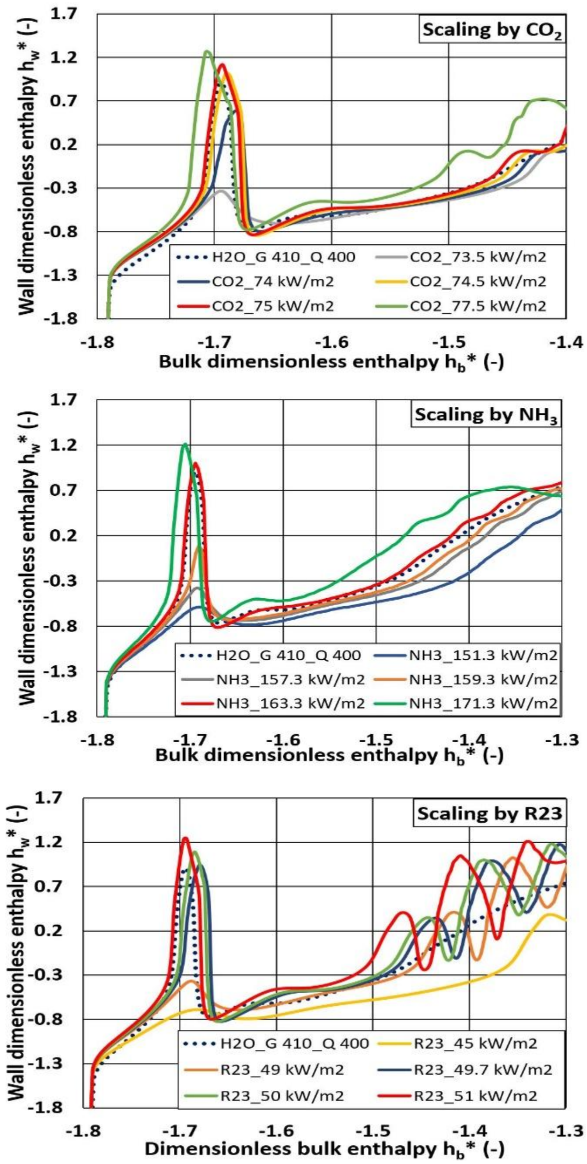


Figure 7. Iterations on heat flux (Reference G=410 kg/m^{2}s)

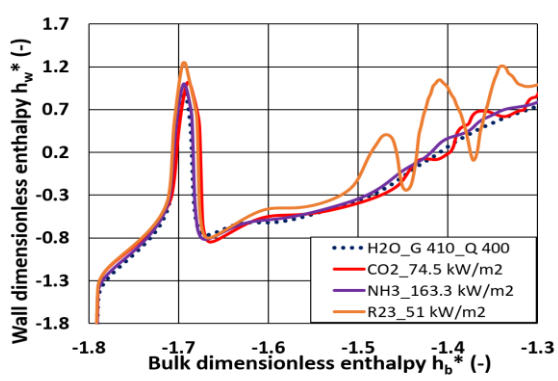


Figure 8. Predictions with the best heat fluxes (Reference G=410 kg/m^{2}s)

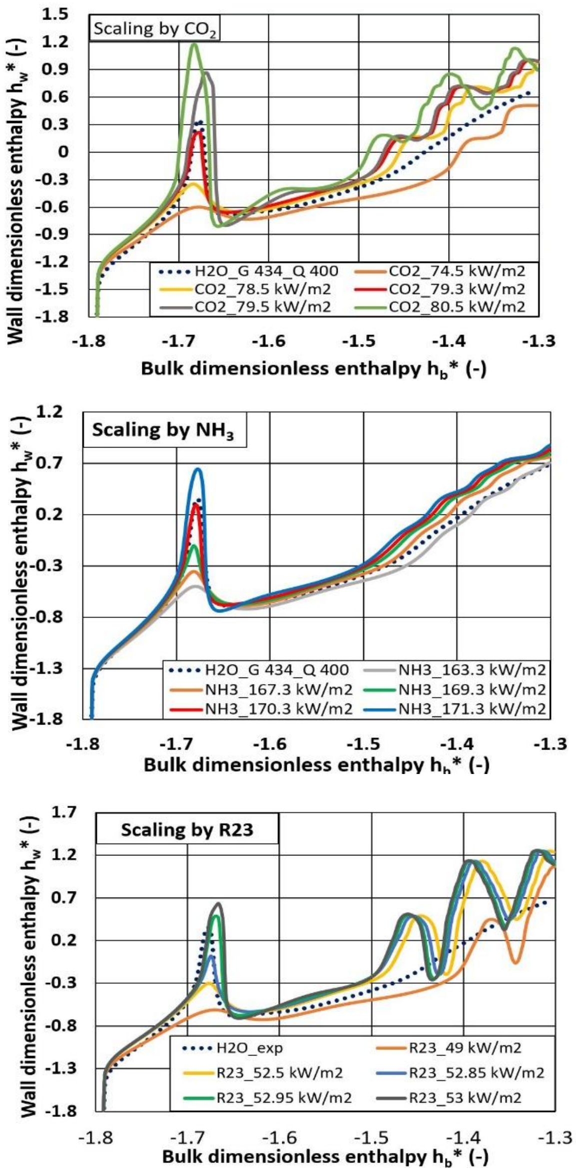


Figure 9. Iterations on heat flux (G=434 kg/m^{2}s)

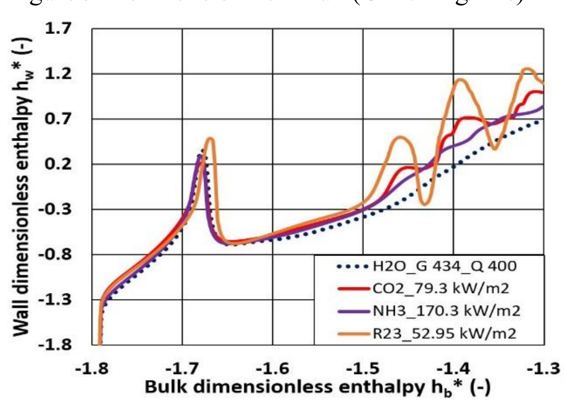


Figure 10. Predictions with the best heat fluxes (Reference G=434 kg/m^{2}s)

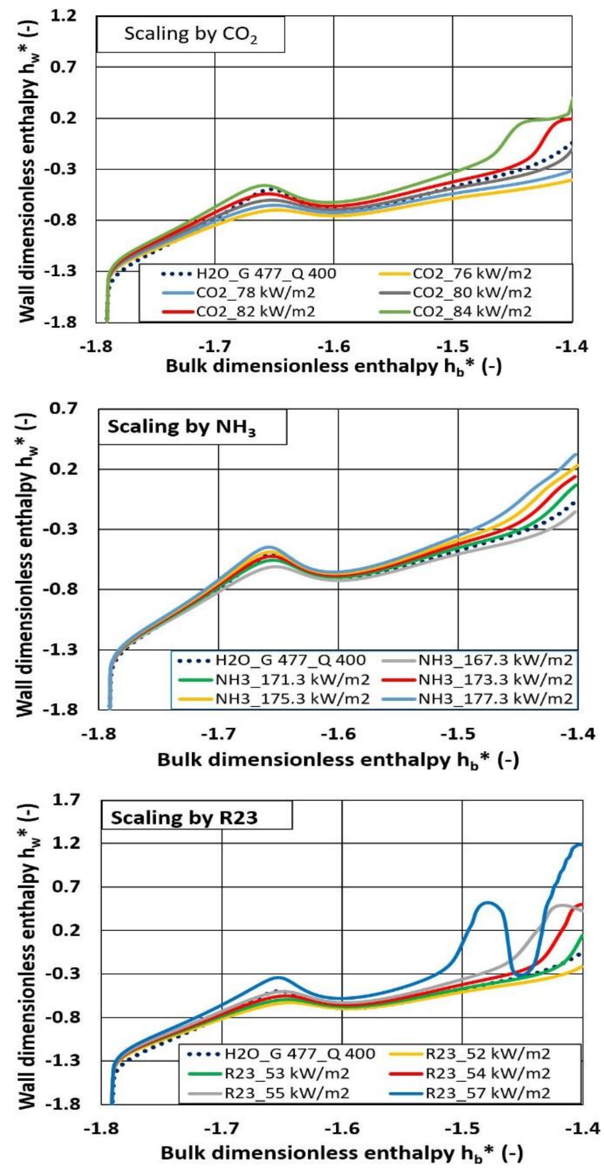


Figure 11. Iterations on heat flux (Reference G=477 kg/m^{2}s)

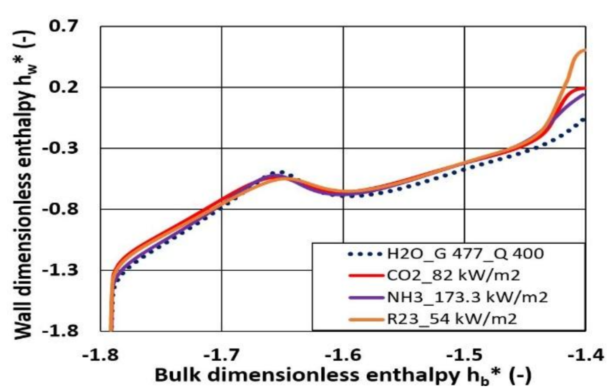


Figure 12. Predictions with the best heat fluxes (Reference G=477 kg/m^{2}s)

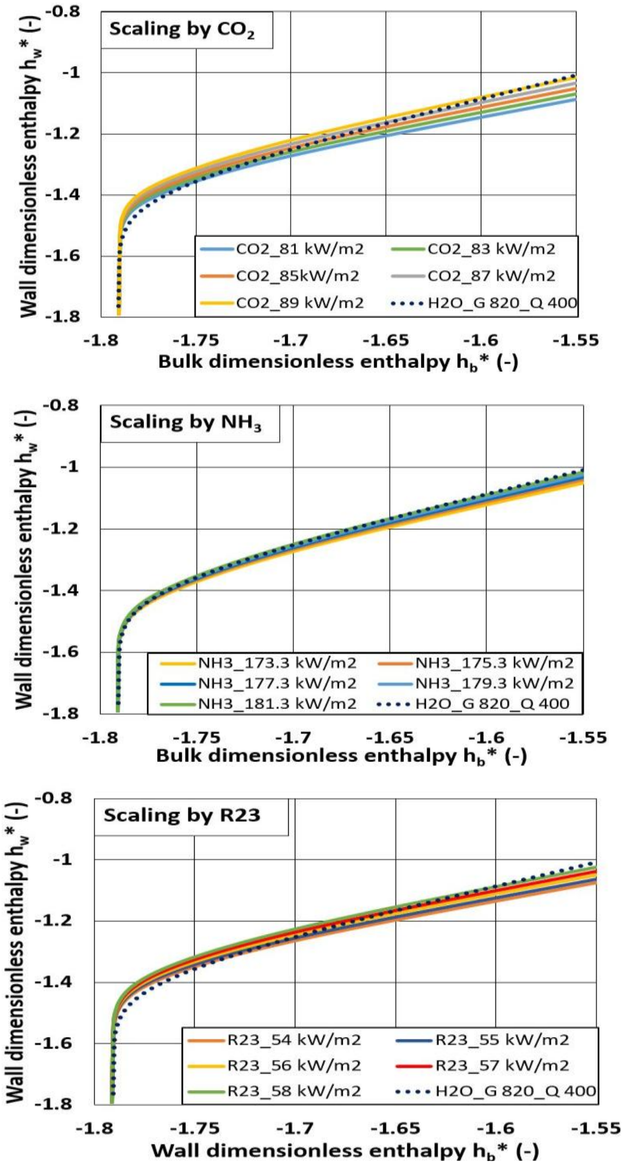


Figure 13. Iterations on heat flux (G=820 kg/m^{2}s)

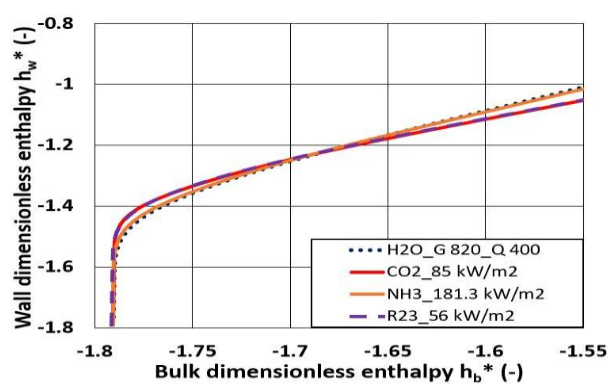


Figure 14. Predictions with the best heat fluxes (G=820 kg/m^{2}s)

CONCLUSION

The application of the similarity theory developed in recent works [8] to the data by Watts [11] allowed achieving further information about its capabilities. In general terms, the main ideas at its basis are confirmed, though it was possible to understand that the sensitivity of the addressed phenomena may always introduce surprises.

A direct or indirect validation of the theory basing on experimental data, by counterpart tests or by developing heat transfer correlations coherent with its rationale, must follow the present arguments, which are presently only supported by theoretical and numerical means.

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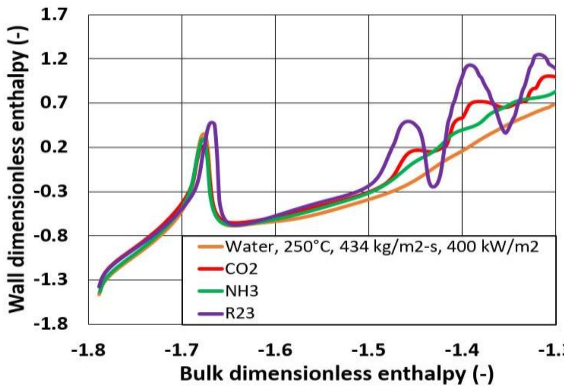
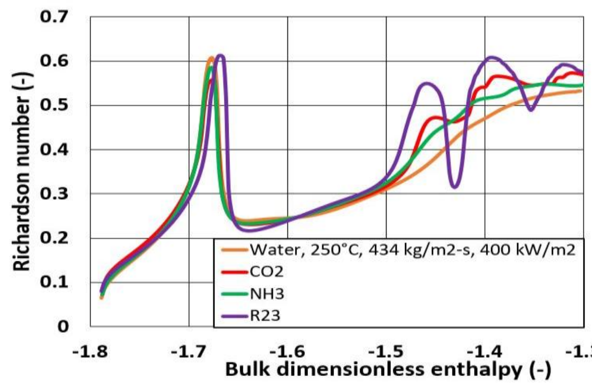
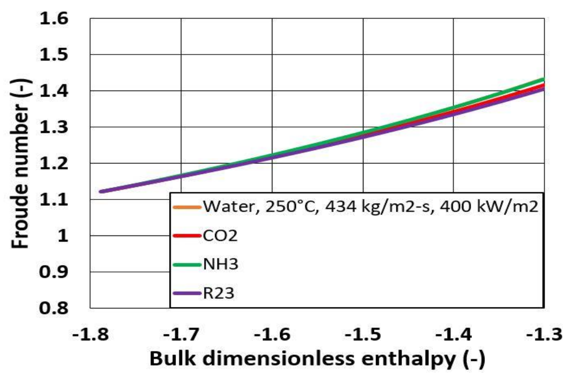


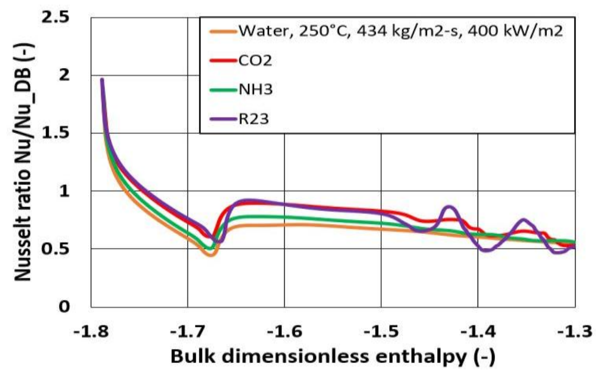
a) Wall dimensionless enthalpy



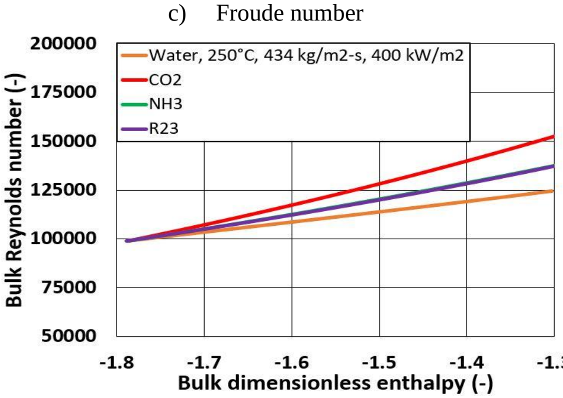
b) Richardson number



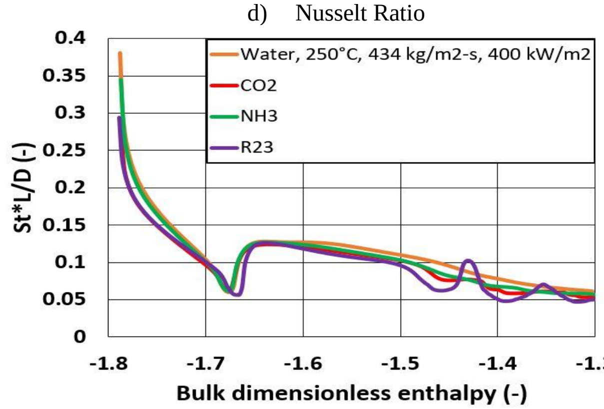
c) Froude number



d) Nusselt Ratio



e) Reynolds number



f) $\overline{St}\left(L/D\right)$

Figure 15. Prediction of the dimensionless numbers along the channel for one of the addressed cases

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