STUDY OF ALGORITHMIC REQUIREMENTS FOR A SYSTEM-TO-CFD COUPLING STRATEGY

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Abstract

Over the last decades, the analysis of transients and accidents in nuclear power plants has been performed by system codes. Though they will remain the analyst's tool of choice for the foreseeable future, their limitations are also well known. It has been suggested that an improvement in the simulation technology can be obtained by "coupling" system codes with Computational Fluid Dynamics (CFD) calculations. This is usually attempted in a domain decomposition fashion: the CFD simulation is only performed in a selected subdomain and its solution is "matched" with the system code solution at the interface. However, another coupling strategy can be envisioned. Namely, CFD simulations can be used to provide closures to a system code.

This strategy is based on the following two assumptions. The first assumption is that there are transients which cannot be simulated by system codes because of the lack of adequate closures. The second assumption is that appropriate closures can be provided by CFD simulations. In this paper, such a coupling strategy, inspired by the Heterogeneous Multiscale Method (HMM), is presented. The philosophy underlying this strategy is discussed with the help of a computational example.

1. INTRODUCTION

The simulation of the steady-state and transient behaviour of nuclear power plants is a considerable challenge, given their size and their geometrical complexity. Traditionally, this task has been carried out by System Thermal Hydraulics (STH) codes. They make the simulation computationally manageable by modelling the system as an assembly of 0-D and 1-D components. The quantities of interest, namely pressure, velocity and internal energy of water and steam are calculated as the solution of the two-fluid model of two-phase flow. Closures are introduced to describe the exchange of mass, momentum and energy between the wall and the fluid and between the phases.

Regardless the modelling simplifications employed by system codes, they have proved to be a valuable simulation machine and they are, *de facto*, the corner stone of the safety analysis of nuclear power plants. It is, although, clear that they don't represent a perfect simulation tool. Aside from the limitations of the two-fluid model, the shortcomings of the STH codes might be intuitively ascribed to two reasons. The first one is the structural limitation of a 1-D code to simulate phenomena where 3-D effects are of predominant importance; the second is the uncertainty of the closures that provide an average description, at the characteristic length scale of system codes, of phenomena actually taking place on much smaller length scales.

It is tempting to think that these problems could be overcome by the use of Computational Fluid Dynamics (CFD) codes. After all, they can simulate 3-D phenomena on very fine meshes and the increasing availability of cheap computational power makes this perspective even more enticing. Setting aside the issues of the maturity of CFD codes (reliable simulation tool for single phase applications, not yet mature for the analysis multi phase flows), the long calculation times associated with CFD simulations, especially for transient problems, imply that CFD codes can be used to complement STH codes in the analyst's toolkit but not to substitute them entirely.

Over the years, various attempts have been made to couple STH and CFD codes. Strategies and goals have been largely different but, not surprisingly, one common feature is at the basis of all these efforts: the need to limit, as much as possible, the calculations on the CFD side.

The research on coupling strategies between STH and CFD codes has mostly been driven by the need of calculating, in selected components, 2-D or 3-D velocity and temperature profiles. This leads naturally to a coupling technique we refer to as "domain decomposition". A fairly mature effort in this direction, which has produced a coupled RELAP-3D/Fluent code, is due to the work of Weaver et al. (2002), Aumiller et al. (2002) and Schultz and Weaver (2003). The coupled RELAP-3D/Fluent code has been recently used to simulate the flow in the outlet plenum of the Very High Temperature Reactor (Anderson, 2008).

However, a second coupling strategy might be devised, one where the CFD code is used to calculate one or more coefficients needed by the system code. The rationale behind this coupling strategy is that, for some transients, the system code's simulations can be improved by providing appropriate closures obtained from CFD calculations. The domain of the CFD solver is, then, to be restricted to a region around one or more mesh nodes of the system code. The details depend on the particular problem at hand, but the idea is that, for efficiency reasons, the domain of the CFD solver should be as small as possible. Apparently, this situation is similar to the domain decomposition approach.

There are, however, remarkable differences. First, unlike the domain decomposition approach, the system code is used to simulate the whole domain of interest. Then, the system code and the CFD code do not need to be coupled on-the-fly, which is convenient essentially for practical reasons. The coupling of the two codes is simpler, without any need for a message-passing software infrastructure.

Naturally, as in the domain decomposition approach, there is the problem of obtaining initial and boundary conditions for the CFD calculation using the 1-D data provided by the system code. However, in this case, we are not particularly interested in the details of the CFD simulation itself; the goal is, rather, the closure we need to provide to the system code. It is clear that, since it is impossible to determine unique 2-D and 3-D pressure and velocity profiles compatible with the control-volume averaged quantities provided by the system code, several boundary conditions for the CFD code can be built, all equally acceptable from the point of view of the compatibility with the system code solution. Each of these boundary conditions will give rise to a different pressure and velocity profile calculated by the CFD code. This problem is paramount in the domain decomposition approach but not necessarily in our strategy since the particular closure we need to calculate might be not sensitive to the details of the CFD solution.

The final goal of this study is the development of algorithms that enable the system code to decide when a CFD calculation needs to be performed (closure-on-demand). In this paper, however, we will deal only with the least efficient closure-on-demand strategy, one where a correct CFD closure is provided to the STH code at every STH time step.

2. MULTI-SCALE METHODS AND CLOSURE-ON-DEMAND

The coupling between a CFD and a STH code might be interpreted as a multi-scale problem. As a matter of fact, we have to devise a way to exploit a physically more detailed model (CFD) which, for efficiency reasons, can not be extended to the whole system. The latter is more conveniently described by a gross, less accurate (at the component level) code (STH).

In particular, the coupling strategy outlined in the Introduction can be interpreted as an application of the HMM. The key point of the HMM is that the real goal of the calculation is the simulation of the system at the macroscale level. The multi-scale nature of the problem implies that the macroscale solver alone is not sufficient to achieve this goal and, therefore, it must be complemented by the microscale solver. One of the ways to do this, applicable to the STH-to-CFD coupling problem

described earlier, is to use the microsolver to calculate some of the closures needed by the macrosolver.

In more formal terms, let us assume that the macroscale model can be expressed in the form

$$\frac{d\Theta}{dt} = f(\Theta, k(\Theta)), \tag{1}$$

k representing a parameter (closure) which conceptually depends on the macroscale variable Θ, but practically the correct relationship between k and Θ is not known. The idea is to recover this information through a microscale simulation. Starting from a macroscale state Θ_0, an initial condition θ_0 for the microscale solver is built and a microscale simulation of time length δt, or a steady-state calculation if we can assume separation of scales, is performed. The microscale result θ^* is then used to calculate a value of the closure k^*. Finally, the system is evolved at the macroscale level according to

$$\frac{d\Theta}{dt} = f(\Theta, k^*). \tag{2}$$

The essential point for the efficiency of the method is to establish when, during a transient, the microscale simulation is needed. The final goal is to develop algorithms enabling the macroscale solver with the capacity to determine at which time $\bar{t}$ the closure $k(\theta(\Theta(\bar{t})))$ has to be evaluated. We refer to this procedure as "closure-on-demand".

3. PROOF OF CONCEPT CALCULATION

The system code employed in these calculations is RELAP5 3.3 version 3.3hi. The CFD code chosen is Fluent version 6.3.23.

3.1 Description of the Problem

Let us consider the flow of water in the sudden expansion (circular cross section) shown in Fig. 1.

Fig. 1: Geometry of the sudden expansion problem.
The dimensions of the system are: R_1 = 0.5 cm, R_2 = 1.5 cm, L_1 = 3 m, L_2 = 5 m.

Let the outlet pressure p_{out} be constant and equal to the atmospheric value, the temperature T constant throughout the system and equal to 293 K. Starting from a steady-state situation where the inlet relative pressure p_{in} is equal to 45 Pa, we want to simulate the transient behaviour of this system in the case that p_{in} increases linearly as a function of time from $p_{initial}$ = 45 Pa to p_{final} = 105 Pa in a time ΔT (see Fig. 2).

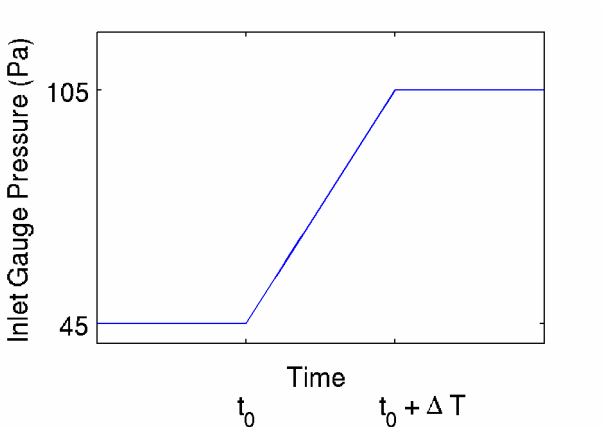

Fig. 2: Inlet boundary condition.

The values of pressure were selected to ensure that the flow stays laminar at all times. Two cases are considered, $\Delta T = 10$ sec and $\Delta T = 5$ sec, referred to as "Transient I" and "Transient II", respectively.

3.2 Microscale Model: CFD

The system is assumed to be axisymmetric, and it is meshed using 150 intervals in the axial direction. 10 and 30 intervals are used in the radial direction in the regions before and after the expansion, respectively. The simulation has been carried out with the unsteady solver, until the system reaches a new steady-state corresponding to the higher value of the inlet pressure, employing a fixed time step of 10^{-3} seconds. Inlet and outlet pressure are given as boundary conditions. The results of the CFD solution are shown in Fig. 3.

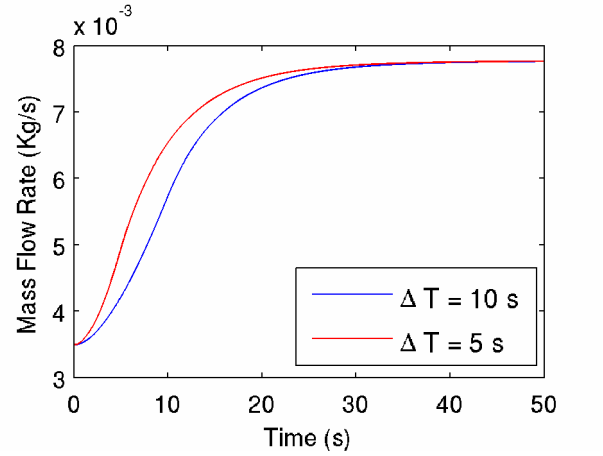

Fig 3: Mass flow rate as a function of time for the Transients I and II (Fluent).

The mass flow rate flowing through the system is determined by the pressure gradient and the hydraulic resistance which, in turn, depends on the viscosity and the velocity gradients. The CFD code provides the value of pressure and the components of velocity at every mesh point. Assuming that the goal of the simulation is just the calculation of the mass flow rate, the use of a CFD code does not seem the most efficient method: its output is much richer than what is really required and, of course, this comes at the cost of longer calculation times. A greater efficiency, related the calculation goals, might be obtained using a system code, provided that the physics of the problem can be correctly modelled.

3.3 Relationship between Macroscale and Microscale Models – Closures

At the scale described by the Navier-Stokes equations (microscale) the mass flow rate is an integral quantity that is calculated by integrating the velocity profile over a cross-section of the channel. The velocity field, in turn, is completely determined by the geometry of the system, the initial condition and the boundary conditions.

At the scale described by the 1-D system code (macroscale), no information on the velocity gradients is available and the mass flow rate is simply determined by the inlet and outlet pressure boundary conditions and the hydraulic resistance. Notice that the concept of hydraulic resistance is entirely macroscopic: it is the effect of the small scale physics which at the 1-D system code level appears in the form of wall friction and localized loss coefficient in the expansion.

Friction factors and localized loss coefficients are, therefore, the *closures* of the macroscale model. With correct closures, the system code would provide the correct result, namely the same mass flow rate value as predicted by the CFD code. In the case of the friction factor in a circular pipe, RELAP5 has, for example, the correct closure for fully developed laminar flow.

For the localized energy loss coefficient in a junction, there are three possible and equally unsatisfactory choices: (i) a built-in sudden expansion coefficient, (ii) a constant, user-defined coefficient, and (iii) a Reynolds number dependent loss coefficient according to the relation

$$K_{loss} = A_F + B_F / \mathrm{Re}^{C_F}, \tag{3}$$

where the positive, constant coefficients A_F, B_F and C_F are user defined and Re is the Reynolds number.

Clearly, no constant value of the energy loss coefficient can represent a correct closure. It is known, in fact, that in the laminar flow regime, energy loss coefficients depend on the Reynolds number even in steady-state conditions.

As far as the functional relation (3) is concerned, it implies that the loss coefficient depends in a unique way on the instantaneous cross sectional averaged value of the velocity, regardless of the system history. However, we cannot expect this to be true during a transient. From a microscale point of view we can say that the details of the velocity field depend on the history of the system. Therefore, for a given value of the Reynolds number, the loss coefficient might assume different values, depending on the characteristics of the transient.

The conclusion is that this seemingly innocuous problem, the calculation of mass flow rate through a sudden expansion, is actually multi-scale: in order to solve it correctly, a system code calculation needs to be supplied with information available only from CFD analysis. Furthermore, the calculation target, the mass flow rate, is an output of the macroscale code, however correct closures for the macroscale model are not available. Thus, this problem can be classified among those that can be treated within the framework of the HMM. The idea is to calculate appropriate loss coefficient through a CFD simulation. The steps needed to establish a closure-on-demand procedure for this problem can be laid out as follows:

1. We must show that if at every time during the transient RELAP5 has access to the correct value of the energy loss coefficient, as calculated from the full reference CFD solution, the system code simulation "matches" the reference solution.
2. We must show that it is possible to match the reference solution even when the correct value of the closure obtained from the complete CFD simulation of the transient is not used at every RELAP5 time step, but just in a selected, limited number of time steps.
3. The development of the actual closure-on-demand procedure is achieved by:

a. Estimating an "acceptable" approximation of the energy loss coefficient at any point during the transient from a CFD calculation, without requiring the simulation of the complete transient.
b. Devising a criterion that guides the choice of the time points when the CFD calculation is invoked.

In this paper we will deal exclusively with the first of the steps above. It still requires performing a complete CFD simulation of the transient and can be thought as the most inefficient form of closure-on-demand procedure, one where the system code "invokes" the calculation of the closure at every time step.

3.4 Macroscale Model: STH

The RELAP5 model is shown in Fig. 4. The channel is simulated by a PIPE component subdivided in N_{tot} = 32 axial volumes of equal length. N and M are the number of volumes upstream and downstream the expansion, respectively.

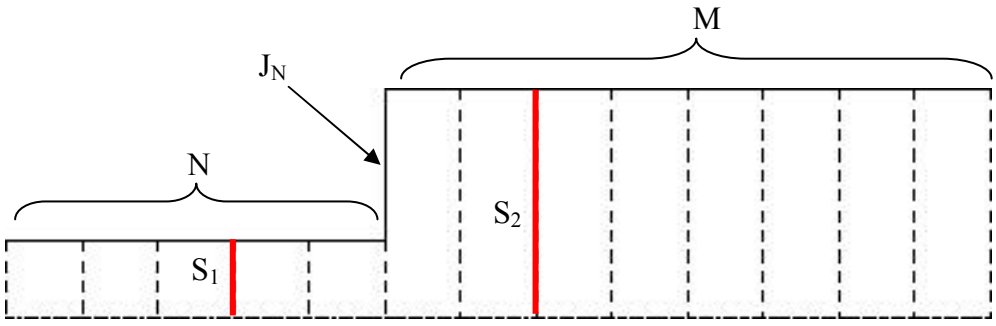

Fig. 4: RELAP5 nodalization of the sudden expansion problem with N = 12, M = 20.
The sudden expansion is modelled by an energy loss coefficient localized in the J_N junction.

The RELAP5 input allows the user to specify a localized energy loss coefficient in any junction of a PIPE component. In the model, the localized loss coefficient is set in the junction J_N, corresponding to the cross-section enlargement. It is calculated as:

$$K_{loss} = 2\hat{E}_v / v_1^2 , \tag{4}$$

v_1 is the velocity in the volume upstream the junction and $\hat{E}_v$ is the energy per unit mass which is dissipated in the volume delimited by the sections S_1 and S_2. $\hat{E}_v$ is evaluated through a Bernoulli-like energy balance:

$$\hat{E}_v = \left(\frac{p_1}{\rho} + \frac{v_1^2}{2} \right) - \left(\frac{p_2}{\rho} + \frac{v_2^2}{2} \right). \tag{5}$$

It is understood that the footers "1" and "2" refer to the surfaces S_1 and S_2 respectively, v is the cross-section averaged value of velocity and ρ is the fluid density. The pressure and velocity values in equation (5) are obtained from the CFD simulation of the same transient.

Notice that two contributions determine the value of $\hat{E}_v$ given by equation (5): the losses due to the sudden expansion and those due to the wall friction between the sections S_1 and S_2. Therefore, in the

RELAP5 model, the flow is assumed frictionless between these two sections, as the wall friction is already accounted for in the formulation of $\hat{E}_v$.

3.5 Steady-State Calculation

First, two steady-state calculations have been performed, corresponding to constant values of the inlet pressure, equal to $p_{initial}$ and p_{final}, respectively. The RELAP5 calculations used a constant value of the energy loss coefficient evaluated from the Fluent simulation according to the procedure described in the previous sub-section. The results are presented in Table 1.

Table 1: Steady-state mass flow rates calculated by Fluent and RELAP5.

Inlet Pressure	Fluent (kg/s)	RELAP5 (kg/s)	Error (%)
$p=p_{initial}$=45 Pa	$3.501 \cdot 10^{-3}$	$3.439 \cdot 10^{-3}$	1.77
$p=p_{final}$=105 Pa	$7.765 \cdot 10^{-3}$	$7.830 \cdot 10^{-3}$	0.84

As it is implied by the above discussion, the steady-state RELAP5 calculations are performed under the constraint that the energy dissipation in the area of the system delimited by S_1 and S_2 is the same as the one obtained by the Fluent calculation. Regarding the discrepancy between the steady-state results provided by the two codes, we mention two possible sources of errors. The first one is the wall friction upstream S_1 and downstream S_2; it is correctly evaluated by RELAP5 only if the flow is fully developed, and we can expect that this requirement is not met, at least in region adjacent to the inlet. The second source of error is in the formulation of the energy balance (5). It should be, more correctly, substituted by the expression

$$\hat{E}_v = \left(\frac{p_1}{\rho} + \frac{1}{2} \frac{< v_1^3 >}{< v_1 >} \right) - \left(\frac{p_2}{\rho} + \frac{1}{2} \frac{< v_2^3 >}{< v_2 >} \right). \tag{6}$$

In the previous expression v_1 and v_2 indicate the velocity profiles on S_1 and S_2 and the operator "< >" indicates cross section average.

3.6 Transient Calculations

The relation between the energy loss coefficient calculated according to (4) and (5) and the Reynolds number evaluated upstream the expansion for Transient I is shown in Fig. 5.

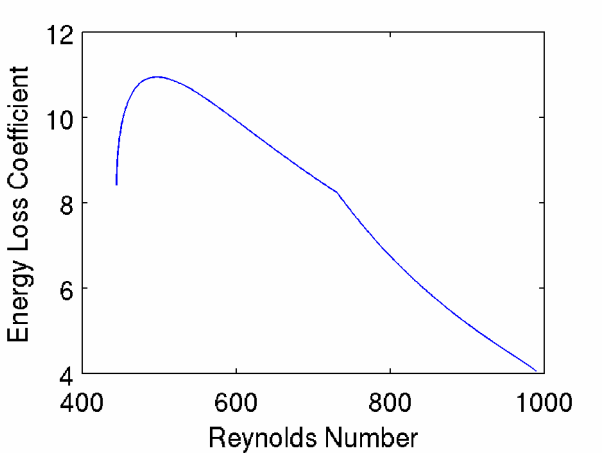

Fig. 5: Energy loss coefficient as a function of the Reynolds number for Transient I.

The discontinuity in the first derivative happens at the same time as the inlet pressure reaches its maximum value. We remark that the correlation (3) implies that $dK_{loss} / d\,\mathrm{Re} < 0$, so it is obviously

unable to reproduce the pattern shown in Fig. 5. This, of course, has an impact on the overall fidelity of RELAP5's simulation. Fig. 6 shows the comparison between the Fluent reference solution and a RELAP5 calculation performed using the formulation (3). The value of C_F has been set to 1.0, and the constants A_F and B_F are the solutions of the linear system

$$\begin{cases} A_F + B_F / \mathrm{Re}_{initial,ss} = K_{initial,ss} \\ A_F + B_F / \mathrm{Re}_{final,ss} = K_{final,ss} \end{cases} . \tag{7}$$

$\mathrm{Re}_{initial,ss}$ is the Reynolds number in the channel obtained from a steady-state CFD calculation performed using a constant value of the inlet pressure equal to $p_{initial}$. $K_{initial,ss}$ is the corresponding energy loss coefficient. Similarly, $\mathrm{Re}_{final,ss}$ and $K_{final,ss}$ refer to the steady-state calculation with inlet pressure p_{final}.

As observed before, in order to establish a closure-on-demand procedure, we must show that, if a correct closure is available, RELAP5 can substantially improve the result presented in Fig 6. Such a closure is obviously the one plotted in Fig. 5. Since the RELAP5 input does not allow to specify loss coefficients as a user defined functions of the Reynolds number, the function shown in Fig. 5 has been hard coded in the source of a custom compiled version of RELAP5 in the form of a table K_{loss} vs. Reynolds number. The correct energy loss coefficient is, thus, evaluated on-the-fly by linear interpolation from the table values. The comparison between the mass flow rate calculated in this way and the reference solution is shown in Fig 7.

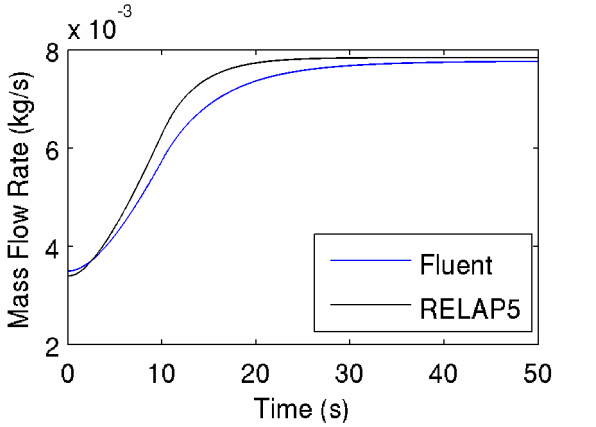

Fig. 6: Comparison between Fluent and RELAP5 solution for Transient I. RELAP5 uses the correlation $K_{loss} = A_F + B_F \cdot \mathrm{Re}^{-1.0}$.

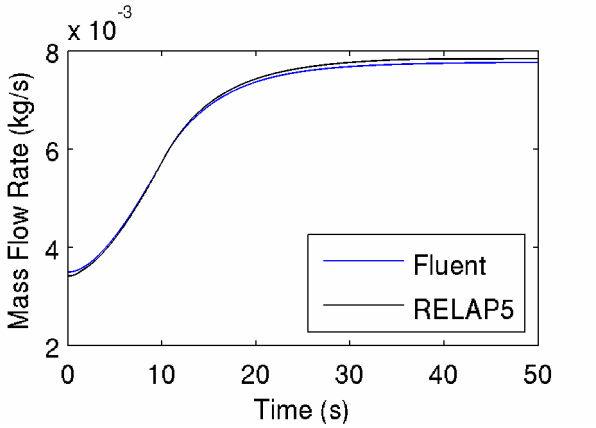

Fig. 7: Comparison between Fluent and RELAP5 solution for Transient I. RELAP5 uses a look up table derived by Fig. 5 to calculate K_{loss}.

The procedure outlined above has been repeated for the second transient with faster pressure ramp (Transient II). Starting from the initial steady-state, the inlet pressure reaches the final value in 5 seconds. The relation between the energy loss coefficient and the Reynolds number for this particular transient is shown in Fig. 8.

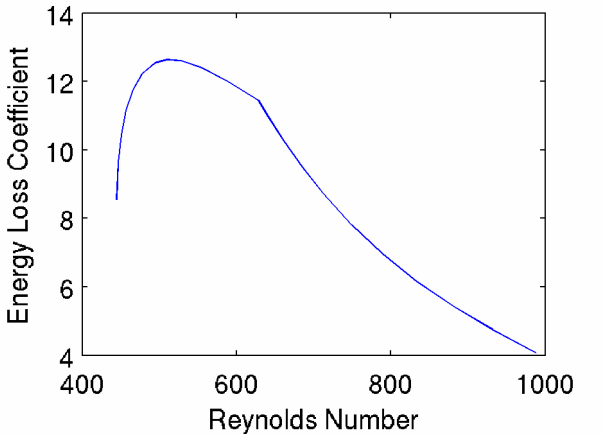

Fig. 8: Energy loss coefficient as a function of the Reynolds number for Transient II.

Fig. 9 and Fig. 10 show the comparison between the reference Fluent solution and the RELAP5 solution with the closure $K_{loss} = A_F + B_F \cdot \mathrm{Re}^{-1.0}$ and the "correct" one, respectively.

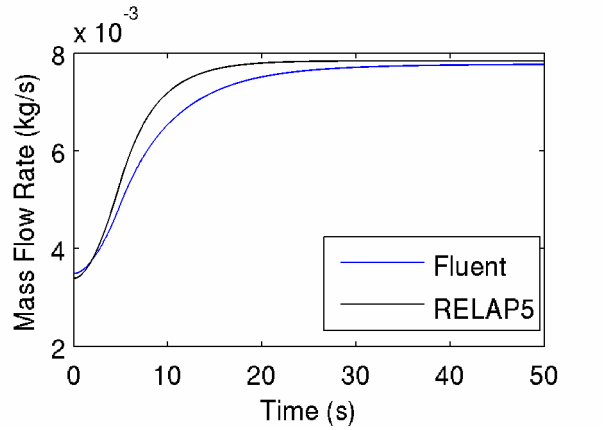

Fig. 9: Comparison between Fluent and RELAP5 solution for Transient II.
RELAP5 uses the correlation $K_{loss} = A_F + B_F \cdot \mathrm{Re}^{-1.0}$.

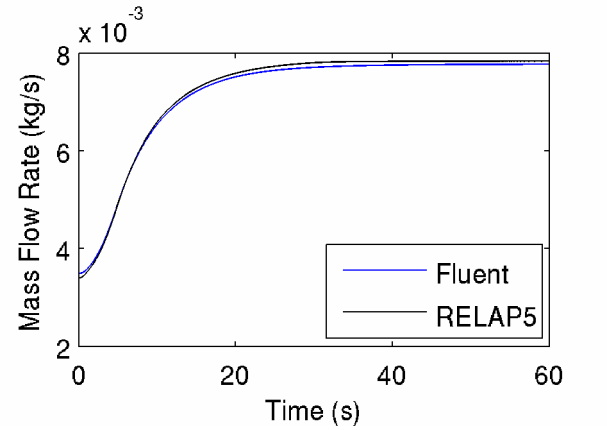

Fig. 10: Comparison between Fluent and RELAP5 solution for Transient II. RELAP5 uses a look up table derived by Fig. 8 to calculate K_{loss}.

4. CONCLUSIONS

The system code RELAP5 and the CFD code Fluent were used to present a STH-to-CFD coupling procedure where a CFD code provides closures to a STH code. This strategy can be related to a popular multiscale framework, namely the HMM. In order to save computational cost, it is necessary to devise algorithms enabling the STH code the capacity to decide when during a transient a CFD simulation has to be performed. A first step in this direction has been taken. In this paper it has been shown that for a particular sample problem, in the most favourable condition when a reference CFD solution is entirely known, it can be used to calculate closures which substantially improve the solution of the STH model.

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