

# On the use of stimulated thermocapillary currents and virtual walls as computational tools for natural convection simulation in enclosed spaces

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A new, alternative approach is proposed for natural convection simulation by means of stimulated thermocapillary currents created by virtual walls. In contrast to the well-known effective thermal conductivity model, in the proposed approach it is the mass motion due to the convective currents which is intended to be simulated and the heat flux is a consequence of such flows. As a result, no a priori knowledge of the Nusselt number is needed and thus the approach is more suitable for complex geometries. Utilizing a simplified physical model and the definition of hydraulic diameter, a generalized expression for enclosed geometries is derived which offers thermal engineers a powerful analysis tool that can use virtual walls with an associated fictitious Marangoni stress for pre-screening and estimation of Nusselt numbers.

**Keywords.** *Natural convection, Effective thermal conductivity, Thermocapillary convection, Computational Fluid Dynamics (CFD)*

## I. INTRODUCTION

Physical enclosures are frequently encountered in practice, and heat transfer through them is of practical interest [1–6]. However, heat transfer in enclosed spaces is complicated by the fact that the fluid in the enclosure, in general, does not remain stationary. For example, in a vertical enclosure, the fluid adjacent to the hotter surface rises and that adjacent to the cooler one falls, establishing rotatory motion (natural convection) within the enclosure that enhances heat transfer. Over the years, several methods have been proposed for the simulation of natural convection, and among them the most popular extension is the use of an effective diffusivity term (effective thermal conductivity) to convert the effects of convection into pure conduction [7, 8]. However, although such an approach offers a viable representation of heat transfer by natural currents, it has an important associated disadvantage. It is therefore worthwhile to briefly review the traditional effective diffusivity method to identify this weakness and then propose an alternative approach which can be used to overcome it.

### A. The effective thermal conductivity model

When the Nusselt number  $\mathbf{Nu}$  is known, the rate of heat transfer  $\dot{Q}$  through an enclosure can be determined

from [9]:

$$\dot{Q} = hA_s(T_1 - T_2) = \kappa \mathbf{Nu} A_s \frac{T_1 - T_2}{L} \quad (1)$$

where  $T_1 - T_2$  is the temperature difference over a distance  $L$ ,  $A_s$  is the area, and the heat transfer coefficient  $h$  is related to the thermal conductivity  $\kappa$  through the definition of the Nusselt number:

$$\mathbf{Nu} = \frac{hL}{\kappa} \quad (2)$$

The rate of steady heat conduction  $\dot{Q}_{\text{cond}}$  across a layer of thickness  $L_c$ , area  $A_s$ , and thermal conductivity  $\kappa$  is:

$$\dot{Q}_{\text{cond}} = \kappa A_s \frac{T_1 - T_2}{L_c} \quad (3)$$

where  $T_1$  and  $T_2$  are the temperatures on the two sides of the layer.

By comparing Eqs. (1) and (3) it can be seen that the convective heat transfer in an enclosure is analogous to heat conduction across the fluid layer in the enclosure, provided that the thermal conductivity  $\kappa$  is replaced by  $\kappa \mathbf{Nu}$  [9]. In other words, the effective thermal conductivity model says: *the fluid in an enclosure behaves like a fluid the thermal conductivity of which is  $\kappa \mathbf{Nu}$  as a result of convection currents.* That is:

$$\kappa_{\text{eff}} = \kappa \cdot \mathbf{Nu} \quad (4)$$

However, as is readily apparent, this effective conductivity model has a serious weakness which limits its applicability in certain circumstances, namely: *it assumes a priori knowledge of the Nusselt number.*

This weakness is somewhat paradoxical, because, in many instances, it is precisely the value of the Nusselt

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number that is sought. So, for example, in attempting to apply the effective thermal conductivity model in an application with complex or unusual geometry, say, in the field of microelectronics, where it might be very difficult to find in handbooks or the available literature a standard Nusselt number correlation for the specific design under consideration, the thermal engineer will need to exercise their judgement in deciding on the most appropriate correlation in order to define the effective thermal conductivity in Eq. (4).

In order to address this problem, in this paper, an alternative method is proposed that makes use of artificially induced thermocapillary flow associated with virtual walls which will promote a mass flow similar to that produced by gravity. The proposed method could be a powerful pre-screening tool for thermal engineers by which to obtain preliminary information about the Nusselt number correlation, and thus to define an effective thermal conductivity. In the next section, we discuss briefly the fundamentals of the proposed approach.

### B. Thermocapillary convection as a simulated induced flow

Marangoni convection occurs when the surface tension of an interface depends on the concentration of a species or on the temperature distribution. In the case of temperature dependence, the Marangoni effect is also called thermocapillary convection. The Marangoni effect is of primary importance in the fields of welding, crystal growth and electron beam melting of metals. For this study it is sufficient to know that as a result of this phenomenon a shear stress is developed in the interface which is caused by the variation of surface tension. The interested reader is referred to reference [10] for further information about this phenomenon and supporting theory.

Within the framework of this kind of convection, a shear stress  $\tau_\sigma$ , which is applied at the wall, is developed. Its value is given by:

$$\tau_\sigma = \nabla_T \sigma \cdot \nabla_s T \quad (5)$$

where  $\nabla_T \sigma = \frac{d\sigma}{dT}$  is the surface tension gradient with respect to temperature, and  $\nabla_s T$  is the surface temperature gradient.

Two aspects of the relationship in Eq. (5) suggest this as a potential application for one-dimensional/two-dimensional natural convection modeling: first, this shear stress is a one-dimensional effect; and second, the effect is driven by a temperature gradient.

## II. MODEL DESCRIPTION

Although, in order to simulate a fluid flow (in this case a thermocapillary flow) in full detail, it is necessary to describe the associated physics in mathematical terms

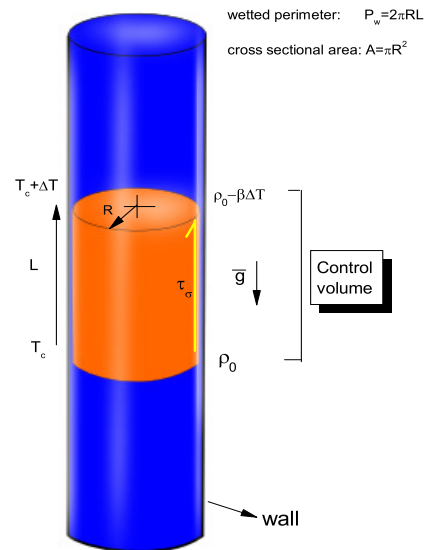


FIG. 1: Control volume used for calculations

through conversation principles, with the use of nonlinear partial or ordinary differential equations to express these principles [11, 12], for preliminary assessment purposes a simple model based on momentum balance is preferable and may be sufficient.

Let us consider a control volume, as depicted in Fig. 1, in order to establish a simplified mathematical model that will allow us to find a suitable expression for the induction of thermocapillary currents in a manner similar to gravitational currents, at least from the point of view of mass transport.

### A. Derivation

First, to analyse flow through the control volume, we need to establish the forces acting on the control volume. The pressure force pushing the liquid through the tube due to the buoyancy forces is given by the change in pressure multiplied by the area:

$$F_g = \rho_o \beta g (\Delta T) \cdot A \cdot L \quad (6)$$

where  $\rho_o$  is the average density of fluid,  $\beta$  is the volumetric coefficient of thermal expansion,  $g$  is the acceleration due to gravity,  $\Delta T$  is the increase in temperature over the length of the control volume,  $A$  is the cross-sectional area, i.e.,  $A = \pi R^2$ , and  $L$  is the length of the control volume.

We can define a (fictitious) Marangoni stress associated with the walls as:

$$F_\sigma = \tau_\sigma \cdot P_w \cdot L \quad (7)$$

where  $\tau_\sigma$  is the Marangoni stress defined previously in Eq. (5),  $P_w$  is the wetted perimeter, i.e.,  $P_w = 2\pi R$ , and  $L$  is again the length of the control volume.

Thus, if we want our induced artificial thermocapillary flow to “replace” the buoyancy-induced flow, this can be accomplished by arranging that:

$$F_\sigma = F_g \quad (8)$$

or, taking into account Eqs. (6) and (7):

$$\tau_\sigma = \rho_o \beta g \Delta T \frac{A}{P_w} \quad (9)$$

A hydraulic diameter  $D_h$  may be defined as [9]:

$$D_h = \frac{4A}{P_w} \quad (10)$$

thus enabling Eq. (9) to be rewritten more compactly as:

$$\tau_\sigma = \rho_o \beta g \Delta T \frac{D_h}{4} \quad (11)$$

Eq. (11) thus allows us to calculate the equivalent fictitious Marangoni stress for any enclosed geometry by means of the calculation of its hydraulic diameter.

However, the most relevant parameter to be calculated for computational simulations is not  $\tau_\sigma$  but rather the surface tension gradient  $\nabla_T \sigma$  associated with the walls, which in computational fluid dynamics (CFD) codes is introduced as a boundary condition for walls. This surface tension gradient can be readily calculated by combining Eqs. (5) and (11), yielding:

$$\nabla_T \sigma = \rho_o \beta g \frac{D_h}{4} \cdot \left[ \frac{\Delta T}{\nabla_s T} \right] \quad (12)$$

If it is reasonable to express the temperature difference in the fluid  $\Delta T$  using an average thermal gradient  $\nabla T$  as

$$\Delta T \approx c_1 \nabla T L \quad (13)$$

where  $L$  is the characteristic length of the system, and  $c_1$  is a scaling constant to take into account the error introduced by the use of an average thermal gradient, then Eq. (12) can be rewritten as:

$$\nabla_T \sigma \approx c_1 \rho_o \beta g L \frac{D_h}{4} \cdot \left[ \frac{\nabla T}{\nabla_s T} \right] \quad (14)$$

Thus, Eq. (14) allows us to define a fictitious surface tension gradient associated with structures which will induce a convective flux similar to a gravitational flux if we know the relationship between the fluid thermal gradient and the surface thermal gradient  $\nabla T / \nabla_s T$ . All the other

parameters in Eq. (14) are either physical or geometrical parameters that are easily determined.

It is also readily apparent that, for computational applications, there is no impediment to the thermal engineer defining virtual walls anywhere in the system. Such walls would only have the function of introducing a Marangoni flux, but they can be defined either with a thermal conductivity equal to that of the surrounding fluid, or, even better, with “shadow conditions” which result in the surface temperature in the virtual wall being identically equal to the immediately surrounding fluid; in other words,  $\frac{\nabla T}{\nabla_s T} = 1$ , and Eq. (14) then reduces to:

$$\nabla_T \sigma \approx c_1 \rho_o \beta g L \frac{D_h}{4} \quad (15)$$

This new proposed concept of virtual walls with an associated Marangoni stress offers a powerful tool for the thermal engineer to use in the preliminary calculation of the Nusselt number for complex systems where the Nusselt correlation is a priori unknown for natural convection computational simulations. These virtual walls can be defined anywhere in the system with a suitably calculated associated Marangoni stress. Fig. 2 shows some schematic examples of the use of such virtual walls for the induction of thermocapillary flows emulating the gravitational flow patterns.

### III. RESULTS AND DISCUSSION

To obtain some idea of the sorts of results predicted by the use of virtual walls with associated Marangoni stresses, some CFD calculations have been performed. The simulations were performed with the **FLUENT-6.3**<sup>®</sup> CFD code. The values of physical properties and operating conditions (e.g., the gravitational acceleration) were adjusted to yield the desired Rayleigh number **Ra**. For the cases presented here, these values were:  $\rho_o = 1000 \text{ kg/m}^3$ ,  $c_p = 1.1030 \times 10^4 \text{ J/kgK}$ ,  $\kappa = 15.309 \text{ W/mK}$ ,  $\eta = 10^{-3} \text{ kg/ms}$ ,  $\beta = 10^{-5} \text{ K}^{-1}$ ,  $g = 6.96 \times 10^{-5} \text{ m/s}^2$ , with the default domain being  $1 \text{ m} \times 1 \text{ m} \times 1 \text{ m}$  in size.

The cases were treated with a pressure-based, segregated, steady solver with Green-Gauss cell-based gradient treatment. The Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm was selected for the pressure-velocity coupling with relaxation factors of 0.3 for pressure, 0.7 for momentum and 1 for energy as the defaults. The pressure was discretized with a standard Rhie-Chow discretisation scheme [13] and Quadratic Upstream Interpolation for Convective Kinematics (QUICK) was chosen as the advection scheme for momentum and energy discretization. The convergence criteria were set for absolute residuals below  $1 \times 10^{-3}$  for all the parameters except energy. ANSYS (2012) recommends a convergence criterion for energy of  $10^{-6}$  [14]. The fictitious Marangoni stress associated with the structure was calculated using Eq. (12) with the constant  $c_1$

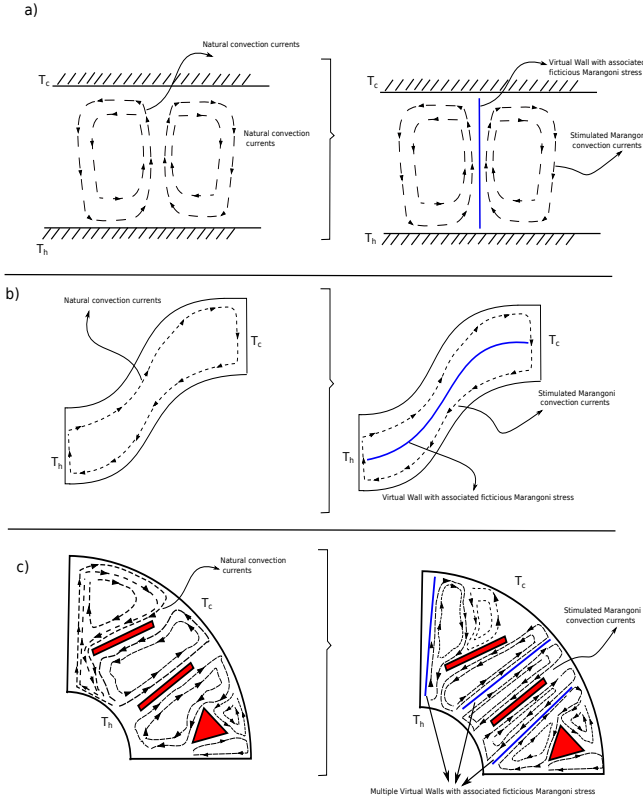


FIG. 2: The use of virtual walls with associated Marangoni stresses. Through the use of virtual walls, Marangoni induced fluxes can be introduced easily. These can be used for the pre-screening of systems in order to obtain a preliminary Nusselt number correlation.

being set initially and then maintained constant for the rest of the calculation for the specified geometry.

Figs. 3, 4 and 5 show the Nusselt number for some generic selected geometries as a function of the Rayleigh number estimated through the use of induced Marangoni fluxes in comparison with the corresponding empirical correlations from experimental data available in the literature [9]. The level of agreement between these correlations and the results given by the approach using induced Marangoni fluxes is apparent and encouraging.

Finally, as a more realistic example, we consider the case of a simple square  $10\text{ cm} \times 10\text{ cm}$  box, as depicted in Fig. 6, but we assume that, for this specific design, there is an arbitrary obstruction, say, a square rhombus, located in the top-right quadrant, as shown. There would be no Nusselt number correlation available in the literature for this specific case, so the calculation of an effective thermal conductivity is not straightforward. However, the thermal engineer could use a virtual wall with an associated calculated Marangoni stress in order to obtain a preliminary relationship for the Nusselt number.

Fig. 7 shows the resulting relationships between Nusselt number and Rayleigh number from a natural convection simulation and using a virtual wall for the geometry depicted in Fig. 6. The Nusselt number relationship for

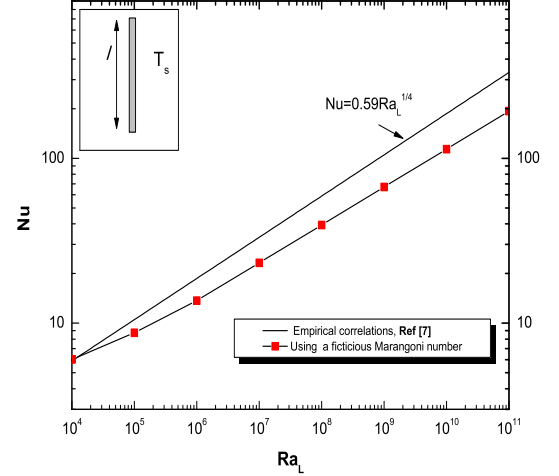


FIG. 3: Comparison between the semi-empirical correlation for the average Nusselt number for natural convection for a vertical plate and that found using fictitious Marangoni fluxes.

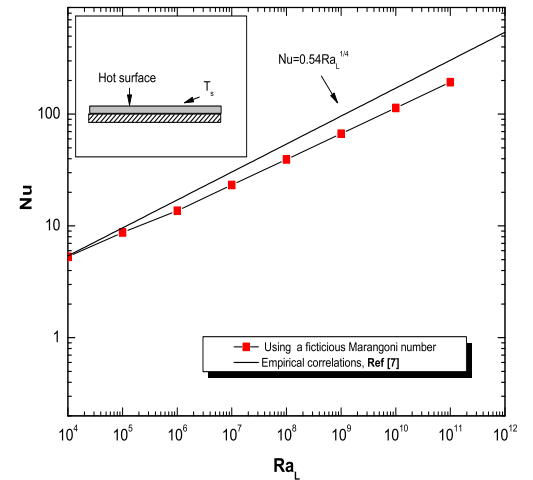


FIG. 4: Comparison between the semi-empirical correlation for the average Nusselt number for natural convection for a horizontal plate with a hot plate upper surface (or a cold plate lower surface) and that found using fictitious Marangoni fluxes.

the simple square box (without the obstruction) is also shown for comparison. The latter will be the ‘best’ correlation available to the thermal engineer from the literature.

For this example, the resulting best fits for the Nusselt number correlations yield the following expressions:

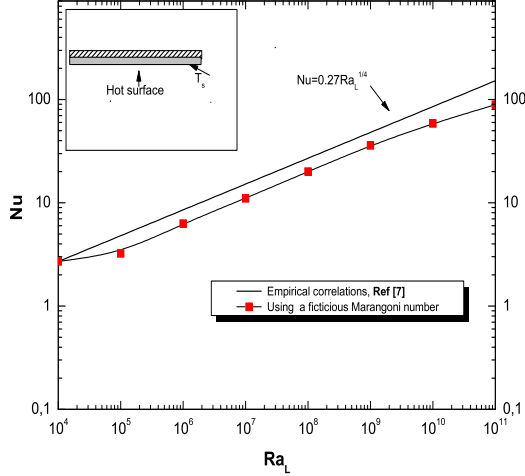


FIG. 5: Comparison between the semi-empirical correlation for the average Nusselt number for natural convection for a horizontal plate with a hot plate lower surface (or a cold plate upper surface) and that found using fictitious Marangoni fluxes.

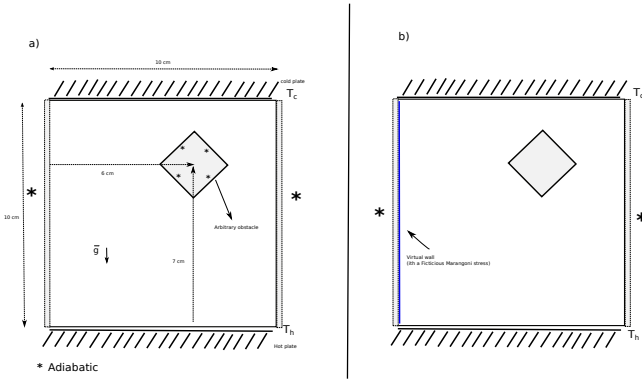


FIG. 6: A square box with an arbitrary obstruction. The purpose of this simulation is to see the Nusselt number obtained through the use of virtual walls in a system where there is no Nusselt number correlation available in the literature.

Using a virtual wall:

$$\mathbf{Nu} = 0.27 [\mathbf{Ra} + 6800]^{0.238} \quad (16)$$

For natural convection:

$$\mathbf{Nu} = 0.27 [\mathbf{Ra} + 2800]^{0.243} \quad (17)$$

The Nusselt number correlation for a square enclosure without the rhombus obstruction available in the literature is:

$$\mathbf{Nu} = 0.27 [\mathbf{Ra}]^{0.25} \quad (18)$$

As is apparent from Fig. 7, the relationship found using the virtual wall approach slightly over-predicts the

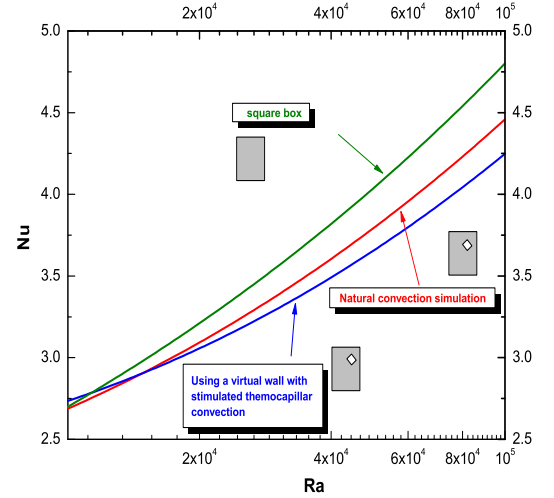


FIG. 7: The Nusselt number from the simulation of the system using natural convection and using an induced thermocapillary flux..

Nusselt number at low Rayleigh numbers and otherwise somewhat under-predicts the Nusselt number for natural convection, but overall it provides a much better estimate of the Nusselt number than that given by square enclosure correlation from the literature.

#### IV. SUMMARY AND CONCLUSIONS

In this paper an alternative approach for natural convection modeling in enclosed spaces has been proposed. This makes use of a stimulated thermocapillary flux associated with a virtual wall. The proposed approach could offer a powerful pre-screening tool for thermal design in complex geometries where a suitable Nusselt number correlation is not available from the literature, and thus it is not possible to obtain a direct definition of an effective thermal conductivity term. Additional research and development are required to explore the potential of this new concept further.

#### NOMENCLATURE

$A$  = cross-sectional area  
 $c_p$  = specific heat capacity at constant pressure  
 $c_1$  = constant  
 $D_h$  = hydraulic diameter  
 $F$  = force  
 $g$  = acceleration due to gravity  
 $h$  = heat transfer coefficient  
 $L$  = characteristic length  
 $\mathbf{Nu}$  = Nusselt number  
 $P_w$  = wetted perimeter  
 $\dot{Q}$  = Heat transfer rate

$R$  = radius  
 $\mathbf{Ra}$  = Rayleigh number  
 $T$  = temperature

### Greek symbols

$\beta$  = thermal expansion coefficient  
 $\rho_o$  = density  
 $\kappa$  = thermal conductivity  
 $\sigma$  = surface tension  
 $\tau$  = Marangoni stress  
 $\eta$  = dynamic viscosity  
 $\nabla$  = gradient

### Subscripts

cond = conduction

$g$  = gravity  
 eff = effective value  
 $s$  = surface  
 $\sigma$  = surface tension

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