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Spatial distribution of mean age and higher moments of unsteady and reactive tracers: Reconstruction of residence time distributions

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ABSTRACT

The purpose of this investigation is to study the spatial distribution of mean age and higher moments of unsteady and reactive tracers. This objective has been achieved by deriving a moment generation transport equation with full generality. Using this equation, it is possible to derive the age and moment equations for other models previously presented in the literature. The novelty of this method relies on a completely general mathematical framework that permits density, velocity or any other fluid variable to be space and time dependent, and the inclusion of multiple inlets to a computational domain. In addition, if a kinetic expression for the appearance/disappearance of the tracer is supplied, the corresponding moments can also be computed accurately. The main results show how the use of this equation along with a reconstruction method for the Residence Time Distribution allows for a decrease of four orders of magnitude in the computational cost required for the obtaining of such distributions in some cases. This result implies that a better understanding of flow features inside vessels and can be gained, and the optimization of such vessels from the viewpoint of the moments of the RTD is possible.

1. Introduction

The concept of age of a fluid particle inside a physical domain is a cross-disciplinary topic in science and engineering. Researchers in areas as diverse as geology and environmental, mechanical and chemical engineering (amongst others) employ this concept to study miscellaneous situations of fluids under flow: the geologist would be interested in the age of a particular water reservoir; the environmental engineer in the age of a contaminant in an enclosure and the mechanical engineer would be focused on the residence time of a fluid inside a vessel. However, all of them employ the same mathematical method to figure out the solution of very different problems.

To determine how a vessel will behave as a heat exchanger, absorber, reactor or other type of process unit, we need to know how the materials flow through the vessel. To do such work in a proper way, it is necessary to measure or compute the velocity at each point of the vessel under study. Before the occurrence of modern measurement techniques in fluids and the onset of Computational Fluid Dynamics (CFD) this was an impractically complex procedure [1].

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Nomenclature

F	tracer mass fraction (step inlet function)
u_i	velocity in the i direction
x_j	coordinate in the j direction
t	time
$\vec{n}$	normal vector
f	tracer mass fraction (impulse inlet function)
$\mathcal{D}$	mass diffusivity of tracer
m_k	kth order moment of the PDF
S	surface
a	first moment of age

Greek

ρ	density
τ	injection time
δ	Dirac delta function
ξ	mixture fraction
Φ	CDF
φ	PDF
ϕ	passive scalar

Subscripts

k	moment of order k
A	refers to a hypothetical surface A
B	refers to a hypothetical surface B

Other symbols

$\mathcal{H}$	Heaviside function
$\bar{x}$	denotes Reynolds average of variable x
$\tilde{x}$	denotes Favre average of variable x
$\hat{x}$	denotes Mixture Fraction average of variable x
$\mathcal{M}_k$	kth order moment of the RTD

Acronyms

CFD	Computational Fluid Dynamics
CDF	Cumulative Distribution Function
PDF	Probability Distribution Function
RTD	Residence Time Distribution

One of the first authors dealing with the concept of age of the fluid was Danckwerts [2]. In his pioneering work, he exemplified the use of distribution functions showing how they can be used to calculate the efficiencies of reactors and blenders, showing the real path of the fluid inside the equipment using tracer experiments. Shortly later, Spalding [3] formalized the problem with the use of transport equations describing the evolution of the distribution functions in time and space from the transport equations of tracers. This approach is very appropriate, because due to the availability of CFD techniques, very developed in the last three decades, the prediction of age of fluids in different situations is possible.

The state of the art in CFD work relying on the concept of age of the fluid is diverse. From the viewpoint of ventilation efficiency, Sandberg [4] developed an equation for the age of the fluid in rooms, and linked this age to different definitions of ventilation efficiency. Essentially, his derivation is similar to that of Spalding. From the viewpoint of chemical engineering, Liu and Tilton [5] derived equations not only for the age, described as the first moment of the Probability Distribution Function (PDF) of the tracer, but for higher moments in steady continuous flows, doing a generalization of the work previously presented by both Spalding and Sandberg. Specifically, they derived a moment generation transport equation for the PDF, which allows the reconstruction of the PDF itself if a reconstruction algorithm is available. This approach is very interesting, since typically the computation time of an unsteady tracer in a computational domain can be very high, or even prohibitive in some situations, and the complete PDF offers significant information. However, the work of Liu and Tilton is restricted to systems with one inlet under steady conditions. Ghirelli and Leckner [6] developed equations for the mean age of the fluid considering unsteady systems with more than one inlet, and applied their method successfully to chemical reactors [7]. However, their approach is limited to the age of the fluid and not expandable towards the higher moments of the PDF, thus the information associated with them is lost using this approach, and the reconstruction of the PDF through its moments not possible.