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Differential-Algebraic numerical approach to the one-dimensional Drift-Flux Model applied to a multicomponent hydrocarbon two-phase flow

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ABSTRACT

This paper presents a numerical investigation of the solution of the steady-state one-dimensional Drift-Flux Model. It is proposed that these simulations, though often based on finite-volume discretizations and iterative sequential procedures, are preferably performed using established numerical methods specifically devised for Differential-Algebraic Equations (DAE) systems. Both strategies were implemented in a computer code developed for simulations of multicomponent hydrocarbon two-phase flows. The SIMPLER semi-implicit algorithm was employed in the solution of the finite-volume discretized model in order to provide comparison grounds with the adaptive BDF-implementation of DAE integration package DASSLC. Based on test simulations of a naphtha two-phase flow under varying heat-transfer conditions, the DAE approach was proved highly advantageous in terms of computational requirements and accuracy of results, both in the absence and presence of flow-pattern transitions. Numerical difficulties arising from the latter were successfully worked around by continuously switching regime-specific constitutive correlations using adjustable steep regularization functions.

1. Introduction

Modeling and simulation of liquid–vapor two-phase flows through pipes, ducts and channels have been motivating intense scientific research for quite a few decades now, partly due to the common occurrence of this scenario in several industrial applications.

Two-phase flow plays, for instance, an important role in the thermal-hydraulics of nuclear water-cooled power reactors, and hence must be understood in sufficient depth to provide satisfactory grounds for their safety analyses (Levy, 1999; Ghiaasiaan, 2008).

Likewise, in the petroleum industry, two-phase flow can be encountered starting at its very extraction, when effluents flowing from producing wells come out as a mixture of oil and gas (Abdel-Aal et al., 2003). In downstream processing, two-phase feeds to distillation columns can be found, as well as additional two-phase lines throughout a given distillation unit. Column instability and tray damage have been reported as resulting from inadequate hydraulics in these lines (Kister, 1990, 2006).

Pipelines for long-distance transportation of natural gas, in turn, frequently carry some liquids as well (water from gas reservoirs or products of condensation due to temperature or pressure changes), thus affecting required pressure drop calculations (Kelkar, 2008; Mokhatab and Poe, 2012).

Putting it in broader terms, Coker (2007) states that two-phase situations exist in almost all chemical process plants, and that small percentages of vapor (7–8% by volume) are already sufficient to alter flow conditions enough that two-phase flow analyses become necessary.

Two-phase flow is analogous to single-phase flow in that its local instant values of densities, velocities, pressure and other field properties all exhibit random fluctuations induced by turbulence and irregular movements of liquid-vapor interfaces (Kleinstreuer, 2003). Detailed predictions capturing such sudden microscopic motions would require solving the governing equations using sufficiently fine grids so as to fully resolve all continuum time and length scales, thus falling in the scope of *Direct Numerical Simulations* or DNS (Tryggvason et al., 2011). In practice, important as though DNS

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Nomenclature

C_0	distribution parameter, [non-dimensional]
d	pipe inner diameter, [m]
D	pipe outer diameter, [m]
f	friction factor, [non-dimensional]
g	gravitational constant, [m/s^2]
h	enthalpy, [J/kg]
h_0	outer convective heat transfer coefficient, [W/(m^2 K)]
k	thermal conductivity, [W/m/K]
NV	number of discretization control volumes
P	pressure, [Pa]
Q	volumetric heat transfer rate, [W/m^3]
T	temperature, [K]
U	overall heat transfer coefficient, [W/(m^2 K)]
v	velocity, [m/s]
$\hat{v}^d ft$	mean drift velocity, [m/s]
x	axial distance, [m]
$\boldsymbol{y}$	Drift-Flux Model primary-variable vector DAE dependent-variable vector
$\langle\rangle_\alpha$	void-fraction weighted area average

Greek symbols

α	void fraction, [non-dimensional]
ρ	density, [kg/m^3]
Γ	volumetric phasic mass generation rate, [kg/(m^3 s)]
θ	pipe inclination angle
σ	surface tension, [N/m]

Subscripts and superscripts

dft	drift
l	liquid phase
m	two-phase mixture
sur	surroundings
v	vapor phase
w	wall

may be as a research tool, its inapplicability in tackling complex engineering problems of practical interest with today's available computational resources is well known. Hence, engineers resort to macroscopic formulations based on proper averaging techniques in which turbulent and interfacial fluctuations are smoothed out, with their effects being statistically accounted for. Solving these averaged equations also bears the advantage of calculating directly the mean values of most key variables, which would be the primary concern even if local instant results could be obtained (Prosperetti and Tryggvason, 2007; Yeoh and Tu, 2010; Ishii and Hibiki, 2011).

Averaged conservation equations of mass, momentum and energy can be obtained for each individual phase and then immediately be put to use together with *macroscopic jump conditions*, in this way giving rise to the *Two-Fluid Model*. Alternatively, both equations in each set can be added together to yield three new field equations governing the flow of the two-phase mixture as a whole, thus laying the foundation for the *Mixture Model*. In this *Drift-Flux Model*, as the latter is most frequently known, the mixture conservation equations must be supplemented with one additional phasic continuity equation to account for concentration changes (Ishii and Hibiki, 2011).

The Two-Fluid Model is said to be the most accurate macroscopic formulation of two-phase systems, and more so when the motions of the two phases are weakly coupled. Though the opposite is usually stated regarding the Drift-Flux Model (i.e., that it is appropriate when the two phases are strongly coupled), the latter has also been reported to effectively represent two-phase mixtures that are weakly coupled locally in practical engineering systems of axial dimensions large enough to translate into sufficient interaction times, just as might be expected in pipelines, ducts and the alike. Moreover, in addition to its smaller formulation in terms of field equations, the Drift-Flux Model also requires much less constitutive models to close the differential system. Given this relative simplicity, and since engineering system analyses are often based upon the response of the total mixture rather than the local behaviors of each phase, the Drift-Flux Model can thus be considered an important means for the simulation of two-phase flows through ducts and channels. Specifically, its one-dimensional formulation naturally lends itself to the geometry at hand, and it is also preferable because the required relative velocity correlation is very difficult to develop in a three-dimensional form (Ishii and Hibiki, 2011).

In steady-state calculations, transient terms drop out and the one-dimensional Drift-Flux Model is then comprised of a set of Ordinary Differential Equations (ODE), albeit supplemented by pertinent algebraic closure relations. Though the numerical solution of suchlike *Differential-Algebraic Equations* (DAE) *Systems* is a well-studied subject and suitable computational codes are quite mature (Brenan et al., 1996; Hairer and Wanner, 1996; Shampine and Reichelt, 1997), a literature survey has shown a rather surprising lack of studies in which two-phase flow averaged equations are solved in this fashion. Instead, such equations have up to now been solved in the finite-volume method framework, with standard finite-volume discretization techniques being often combined with semi-implicit segregated algorithms such as SIMPLE and its variants (Prosperetti and Tryggvason, 2007; Yeoh and Tu, 2010; Talebi et al., 2012; Morales-Ruiz et al., 2012). Zou et al. (2016a,b) recently reported results with the 1-D Drift-Flux and Two-Fluid Models on a staggered grid using both first-order and high-resolution upwind spatial discretization schemes along with the JFNK (Jacobian-free Newton-Krylov) method to solve the discretized non-linear equation system. Abbaspour et al. (2010), on the other hand, used finite difference approximations for the derivatives of a five-equation model and solved the resulting algebraic equations in their pipeline simulations with the Newton-Raphson method.

The present study aims to fill this gap by presenting a theoretical and practical comparison between both numerical approaches. First, based on a thorough side-by-side analysis of their algorithmic strategies, it is proposed that the solution of the steady-state one-dimensional Drift-Flux Model (or any steady 1-D two-phase flow model, for that matter) is preferably pursued through DAE firmly established means over the iterative semi-implicit finite-volume method, as the latter treats one-dimensional and multidimensional formulations in much the same way, thus failing to fully exploit the former's mathematical peculiarity to its full advantage.

Subsequently, it is sought to corroborate the expected gains of the proposed approach, based on the relative performance of both methods. For the sole purpose of these demonstrations, a two-phase multicomponent hydrocarbon mixture is considered to flow through a process pipe. Thermophysical and transport properties are rigorously evaluated at every axial position as functions of local temperature, pressure and phasic molar compositions, thus imposing additional non-linear constraints. A representative finite-volume discretization of the 1-D Drift-Flux Model's conservation equations was carried out on a staggered grid, and the SIMPLER algorithm was programmed to handle pressure-velocity coupling (Patankar, 1980; Versteeg and Malalasekera, 2007). Calculations were also performed using the Backward Differentiation Formulas implemented in DAE-solver DASSL's extended version DASSLC (Brenan et al., 1996; Secchi, 2012), having compared favorably with