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PII: S0098-1354(16)30336-2
DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2016.11.002
Reference: CACE 5590

To appear in: *Computers and Chemical Engineering*

Received date: 17-8-2016
Revised date: 9-10-2016
Accepted date: 2-11-2016

Please cite this article as: Sabine Le Borne, Lusine Shahmuradyan, Fast algorithms for hp-discretized univariate population balance aggregation integrals, *<![CDATA[Computers and Chemical Engineering]]>* (2016), http://dx.doi.org/10.1016/j.compchemeng.2016.11.002

# Fast algorithms for hp-discretized univariate population balance aggregation integrals

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**Abstract**

The efficient numerical simulation of population balance equations requires sophisticated techniques in order to combine accuracy with efficiency. We will focus on the numerical treatment of aggregation integrals that often dominate the overall time in population balance simulations. Following a finite element approach, the density distribution is discretized through a piecewise polynomial of order $p > 0$ on a nested grid that is refined locally toward an arbitrary point. The proposed method conserves mass while reducing the quadratic complexity (in the dimension of the solution space) of the direct computation to an almost linear complexity. The complexity improvement is based on recursion formulas exploiting orthogonality properties of basis functions along with FFT on locally equidistant portions of the grid. We present numerical results for various initial conditions and provide heuristic criteria for the choice of polynomial degree and grid refinement.

*Keywords:* Population balance equation; Convolution; Integro-partial differential equation; Fast Fourier transformation; Nested grids; High order polynomials

## 1. Introduction

Applications of population balance equations (PBE) can be found in a wide range of processes in chemistry and biology, e.g., in crystallization and precipitation of pharmaceutical materials. The solution of population balance equations is a density distribution $f(t, r, x)$ (Ramkrishna (2000)). It yields the density of particles of property $x$ at time $t$ and space $r$. The variable $x$ denotes the property coordinates of the dispersed phase particles. In this paper, the particle mass is considered as particle property. The state of the entire particle population is quantified by a

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