Agglomeration solver FFT

General description

Performs calculation of the agglomeration process in form of birth $B_{agg}(n,v,t)$ and death $D_{agg}(n,v,t)$ terms based on a separable approximation of the agglomeration kernel and a subsequent fast Fourier transformation:

$$\frac{\partial n(v,t)}{\partial t} = B_{agg}(n,v,t) - D_{agg}(n,v,t),$$

$$B_{agg}(n,v,t) = \frac{1}{2}\beta_0 \int_0^v \beta(u,v-u)n(u,t)n(v-u,t)du,$$

$$D_{agg}(n,v,t) = \beta_0 n(v,t) \int_0^\infty \beta(u,v)n(u,t)du$$

- v and u are volumes of agglomerating particles
- $n(v,t)$ is the number density function
- $B_{agg}(n,v,t)$ and $D_{agg}(n,v,t)$ are the birth and death rates of particles with volume v caused due to agglomeration
- β_0 is the agglomeration rate constant, dependent on operating conditions but independent from particle sizes
- $\beta(v,u)$ is the agglomeration kernel describing the agglomeration frequency between particles of volumes v and u, which produce a new particle with the size $(v+u)$
- t is time

The agglomeration kernel $\beta(v,u)$ is represented in a separable form with the separation rank M as:

$$\beta(v,u) = \sum_{i=1}^{M} a_i(v)b_i(u).$$

Then birth and death terms are transformed to:

$$B_{agg}(n,v,t) = \frac{1}{2}\int_0^v \psi_i(v-u,t)\varphi_i(u,t)du,$$

$$D_{agg}(n,v,t) = \psi_i(v,t)\int_0^\infty \varphi_i(u,t)du,$$

$$\psi_i = a_i n$$

$$\varphi_i = b_i n$$

The separation turns the birth rate agglomeration integral into a convolution form $\varphi_i * \psi_i$, which after piecewise constant discretization, is computed based on the convolution theorem

$$\varphi_i * \psi_i = IFFT\big(FFT(\varphi_i) \odot FFT(\psi_i)\big),$$

applying the direct and inverse fast Fourier transformation ($FFT/IFFT$) and the elementwise product $\odot$.

Kernels separation

Kernel	Separation
Constant	$\beta(u,v) = \sum_{i=1}^{1} a_i(v) b_i(u)$ $a_1(v) = 1, b_1(u) = 1$
Sum	$\beta(u,v) = \sum_{i=1}^{2} a_i(v) b_i(u)$ $a_1(v) = v, a_2(v) = 1, b_1(u) = 1, b_2(u) = u$
Brownian	$\beta(v,u) = \sum_{i=1}^{3} a_i(v) b_i(u)$ $a_1(v) = \sqrt{2}, \quad a_2(v) = v^{\frac{1}{3}}, \quad a_3(v) = v^{-\frac{1}{3}},$ $b_1(u) = \sqrt{2}, b_2(u) = u^{-\frac{1}{3}}, b_3(u) = u^{\frac{1}{3}}$
Product, Shear, Peglow, Coagulation, Gravitational, Kinetic energy, Thompson	Approximated by a rank-M separable function $\beta(v,u) \approx \sum_{i=1}^{M} a_i(v) b_i(u)$ using adaptive cross approximation

Requirements

- Solid phase
- Particle size distribution
- Equidistant volume grid for particle size distribution
- Grid for particle size distribution, starting with 0

References

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S. Le Borne, L. Shahmuradyan, K. Sundmacher, Fast evaluation of univariate aggregation integrals on equidistant grids. Computers and Chemical Engineering 74 (2015) 115-127.