

# Contents

<b>1</b>	<b>Fundamentals of Gas-to-Particle Mass Transfer</b>	<b>1</b>
1.1	Introduction to Sorption Modeling	1
1.2	Formulation	2
1.2.1	Governing Equations	2
1.2.2	Non-dimensionalization	4
1.3	Problem Description	6
1.3.1	Assumptions	6
1.3.2	System Parameters	7
1.3.3	Numerical Specifications	8
1.3.4	Simulation Results for Concentration Fields and Gas-to-Particle Mass Transfer	8
1.3.5	Analytical Solution for the Macropore Concentration in the Intermediate Regime	13
1.4	Summary and Conclusions	14
<b>2</b>	<b>Particle Dispersion and Mass Transfer in Turbulent Shear Flows</b>	<b>17</b>
2.1	Strategies for Sorption Modeling in Turbulent Flows	17
2.2	Formulation	19
2.2.1	Fluid Field	19
2.2.2	Particle Field	19
2.2.3	Gas-to-Particle Mass Transfer	20
2.3	Particle Injection Through a Round Nozzle	21
2.3.1	Particle Dispersion	21
2.3.2	Particle Reynolds Number	23
2.4	Multiphase Mixing Layer Transport	24
2.4.1	Physical Parameters	25
2.4.2	Numerical Specifications	26
2.4.3	Fluid Field and Particle Dispersion	27
2.4.4	Mass Transfer	30
2.5	Summary and Conclusions	34

<b>3</b>	<b>LES of Particle Dispersion and Gas-to-Particle Mass Transfer in Turbulent Shear Flows</b>	<b>37</b>
3.1	Introduction	37
3.2	Formulation	38
3.2.1	Fluid Field	38
3.2.2	Particle Field	39
3.2.3	Modeling of the SGS Stress	39
3.2.4	Modeling of the SGS Fluid-Scalar Flux	41
3.3	Evaluation of SGS Closures for LES of Gas-to-Particle Mass Transfer	41
3.3.1	Fluid Field	43
3.3.2	Chemical Transport	46
3.3.3	Performance Assessment	47
3.4	LES of Gas-to-Particle Mass Transfer	49
3.4.1	Assumptions	49
3.4.2	Numerical Specifications	50
3.4.3	Fluid and Species Transport	50
3.4.4	Particle Transport	52
3.4.5	Mercury Adsorption	53
3.5	Summary and Conclusions	55
	<b>References</b>	<b>57</b>

Modeling of Gas-to-Particle Mass Transfer in Turbulent  
Flows

Garrick, S.C.; Bühlmann, M.

2018, XII, 61 p. 33 illus., 15 illus. in color., Softcover

ISBN: 978-3-319-59583-2