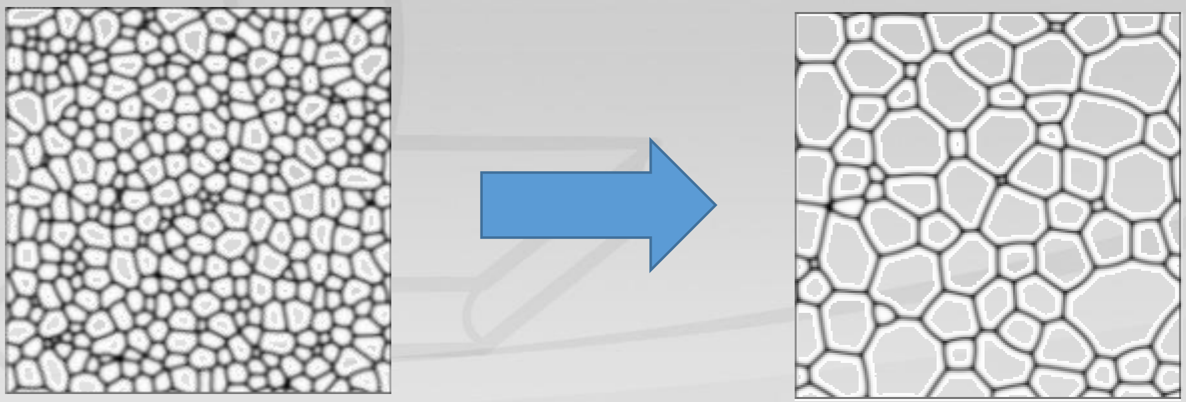
Multi class grain growth model in MatCalc 6

(MatCalc 6.00.0200)

P. Warczok

Grain growth



- Tendency - to minimize:
  - grain surface area
  - specific grain boundary energy

Grain growth kinetics

- General idea: Mobility & Driving force

$$\dot{D} = \frac{dD}{dt} = M P_D$$

$\dot{D}$ - Grain size growth rate

M - Grain boundary mobility

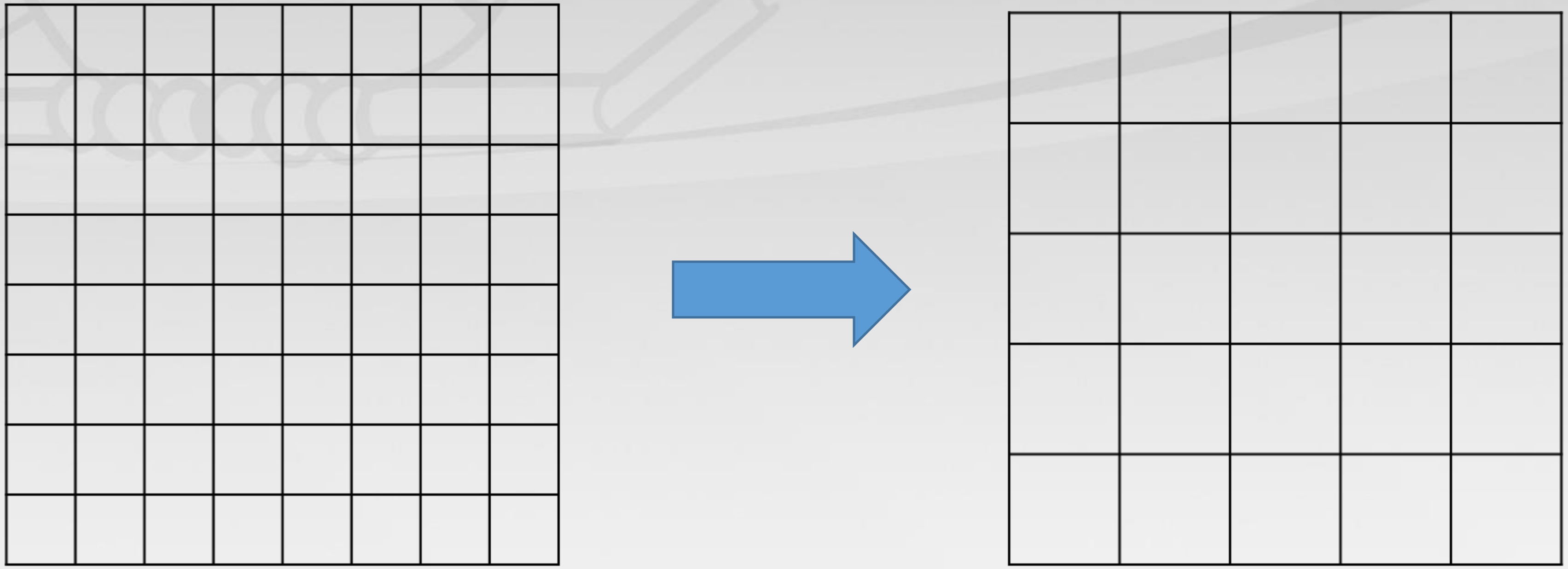
P_D - Driving force/pressure for grain growth

t - Time

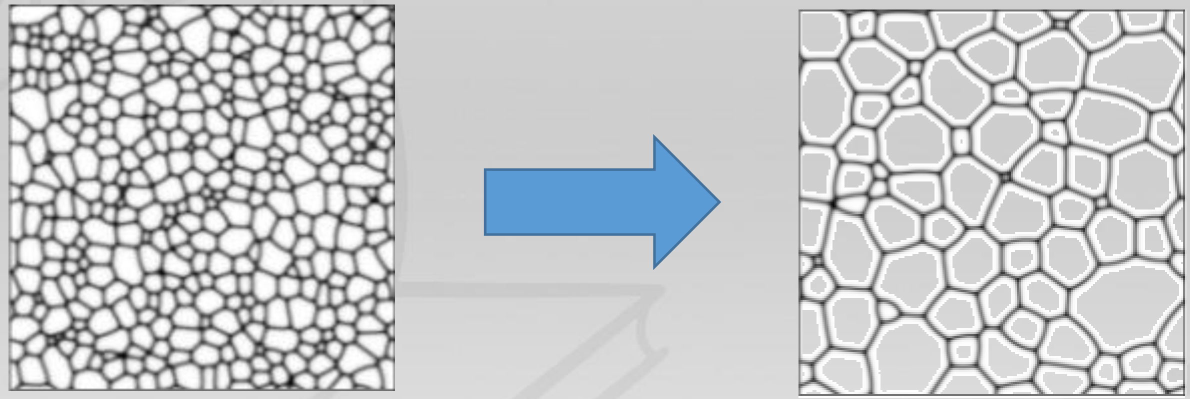
Single class grain growth

- Single quantity: Mean grain size

D_1 D_2



Multi class grain growth

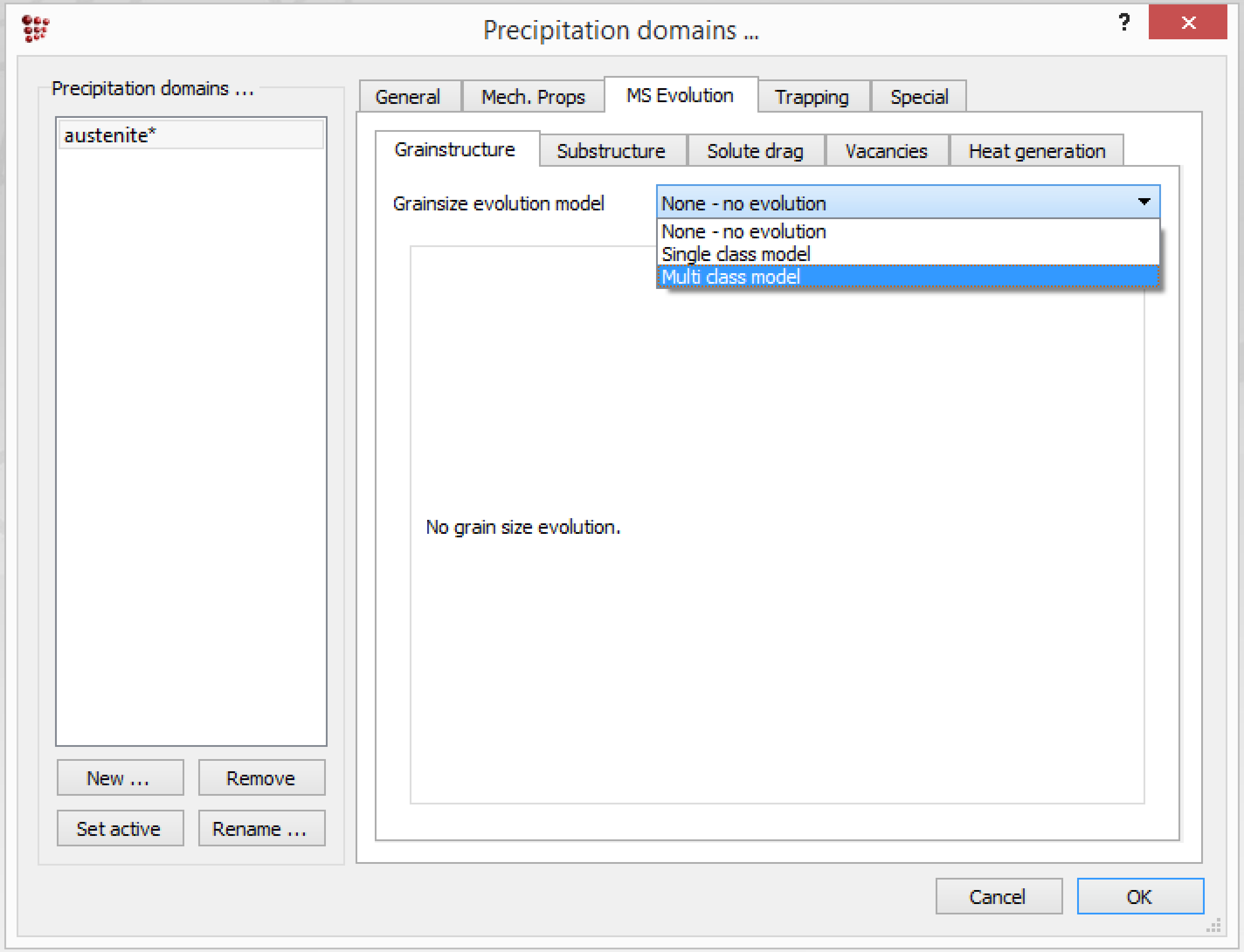


Various grain sizes need to be followed simulatneously…

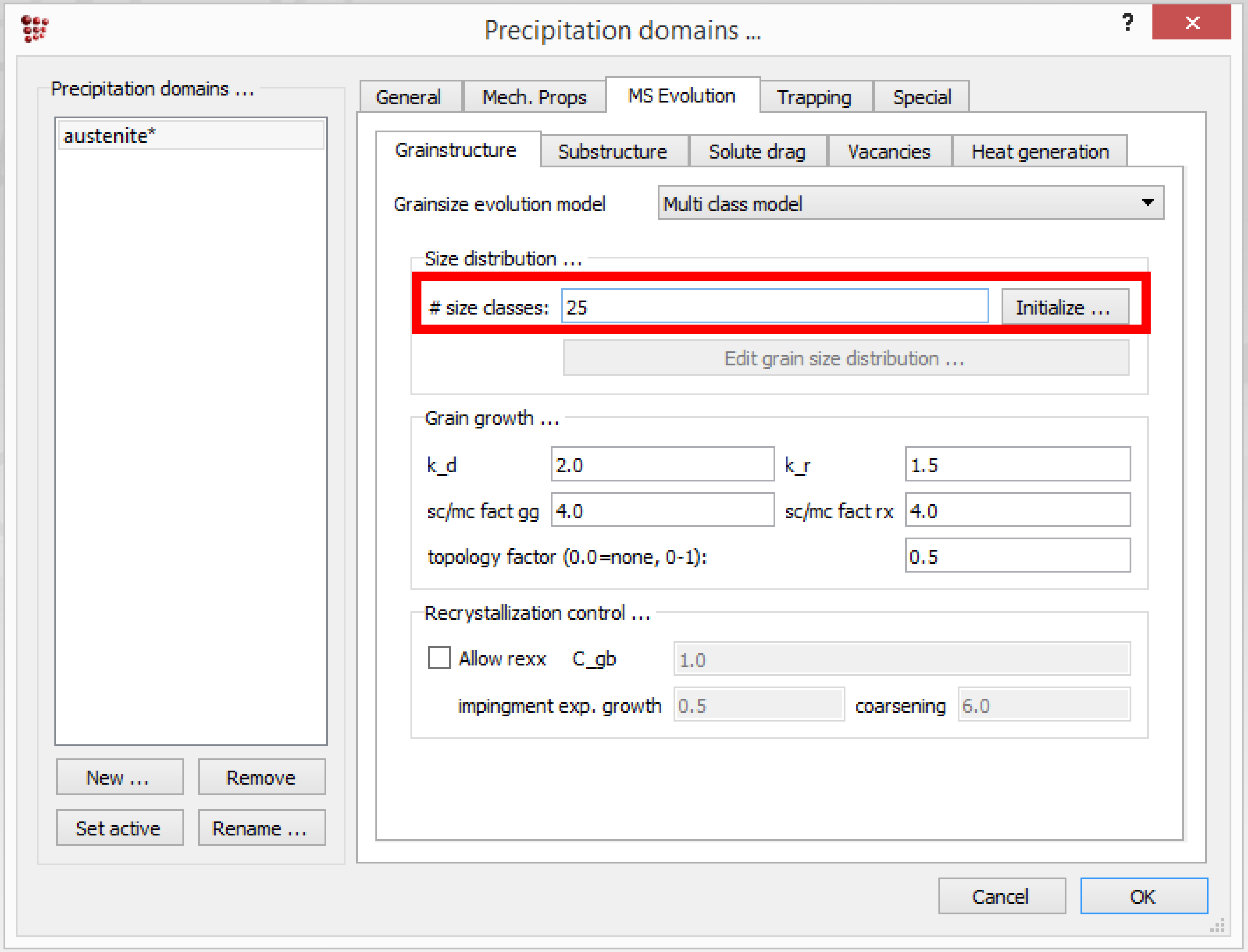
Multi Class Grain Model (MCGM)

- Class representation – as for precipitates
- Each class has identical:
  - size (diameter)
  - accumulated strain
  - dislocation densities
  - subgrain size
  - etc.

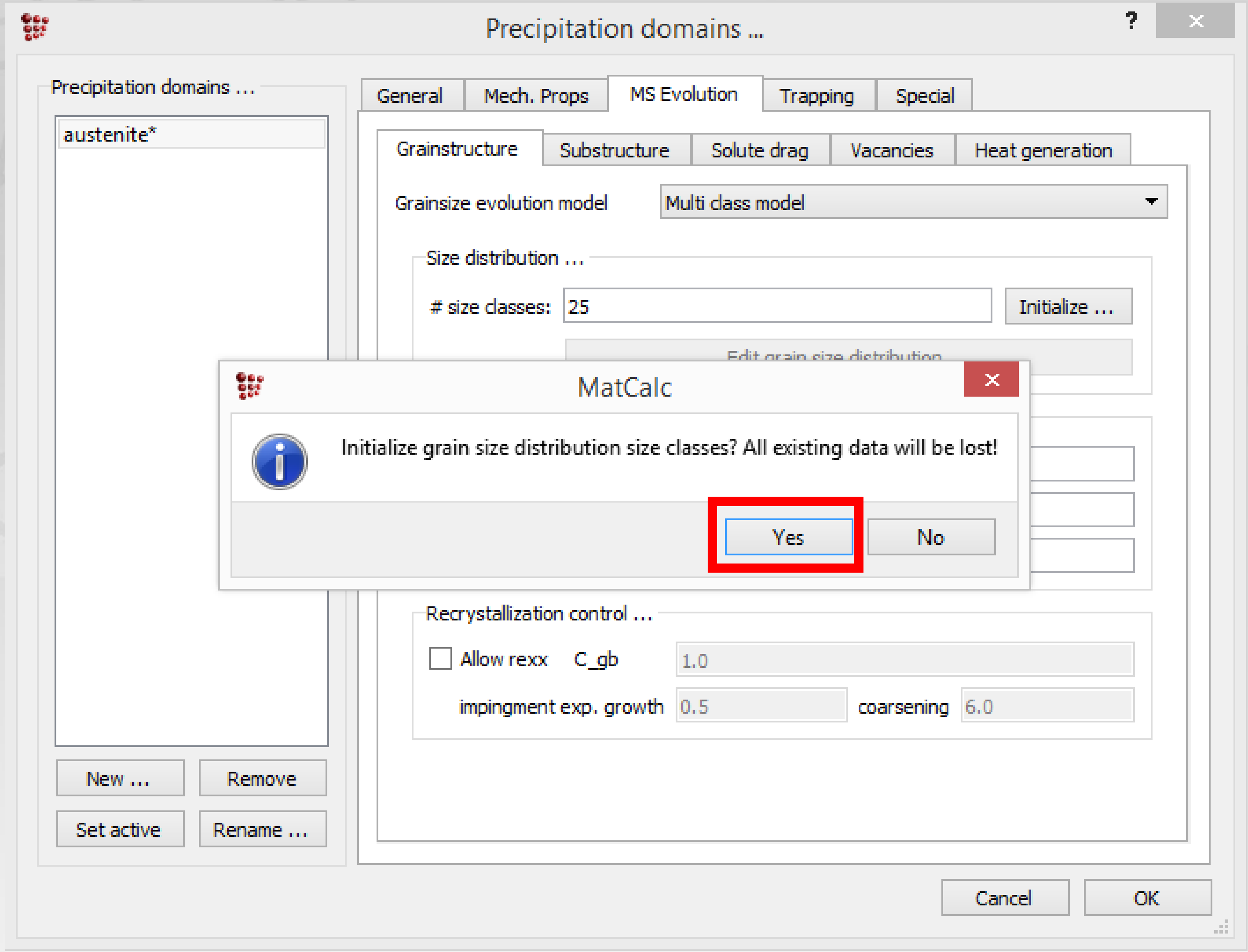
MCGM - selection



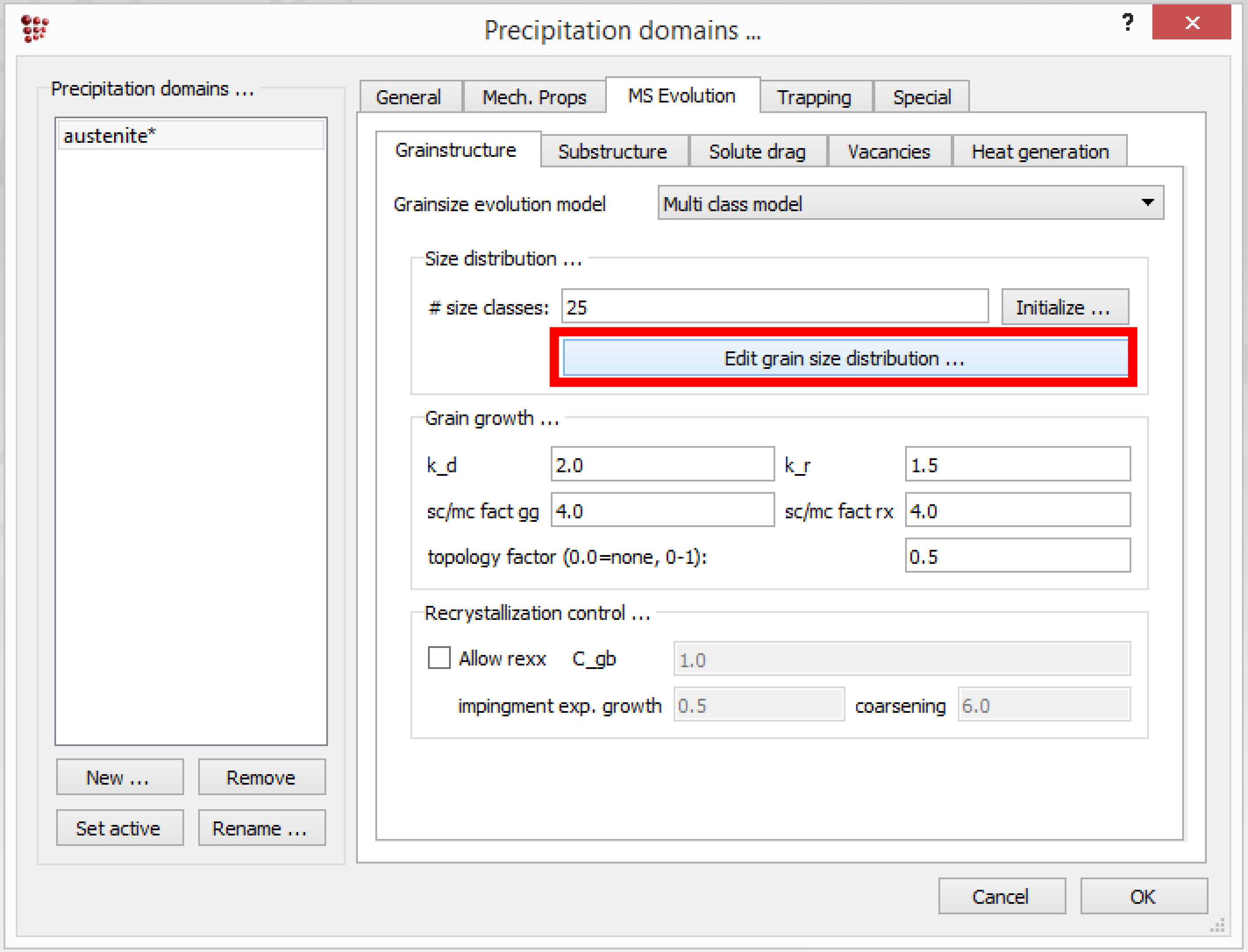
MCGM – class definition



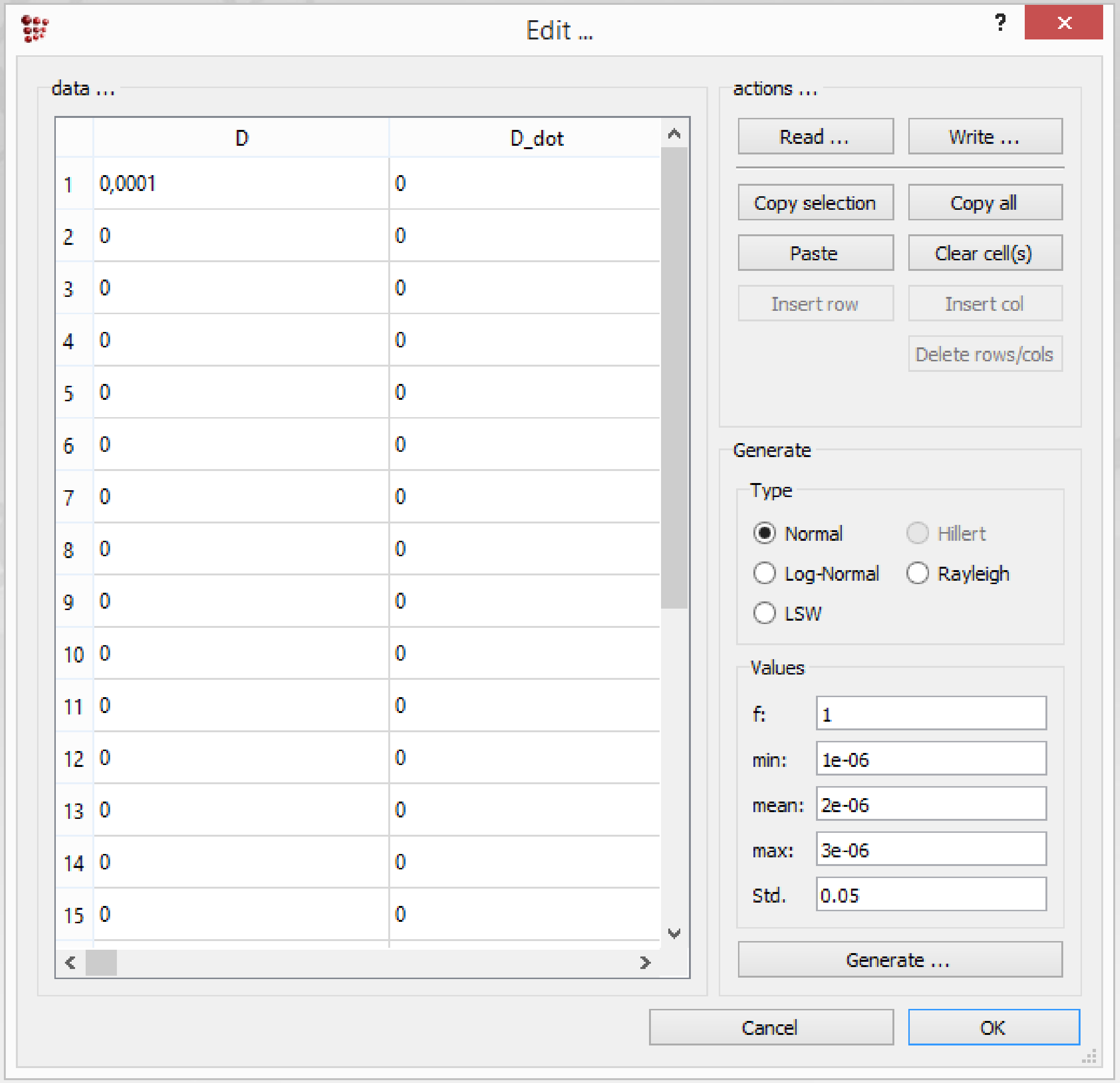
MCGM – class definition



MCGM – class inspection



MCGM – class inspection



MCGM – class inspection

data ...

	D	D_dot	N	X_N_av	acc_eps	dd_ex_internal	dd_ex_wall	dd_ex_int_dot	dd_ex_wall_dot	dd_ex_internal_sat	dd_ex_wall_sat	sgd	sgd_dot	sgd_sat	sgb_misorientation
1	0,0001	0	19098...	1	0	0	0	0	0	0	0	0,0001	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

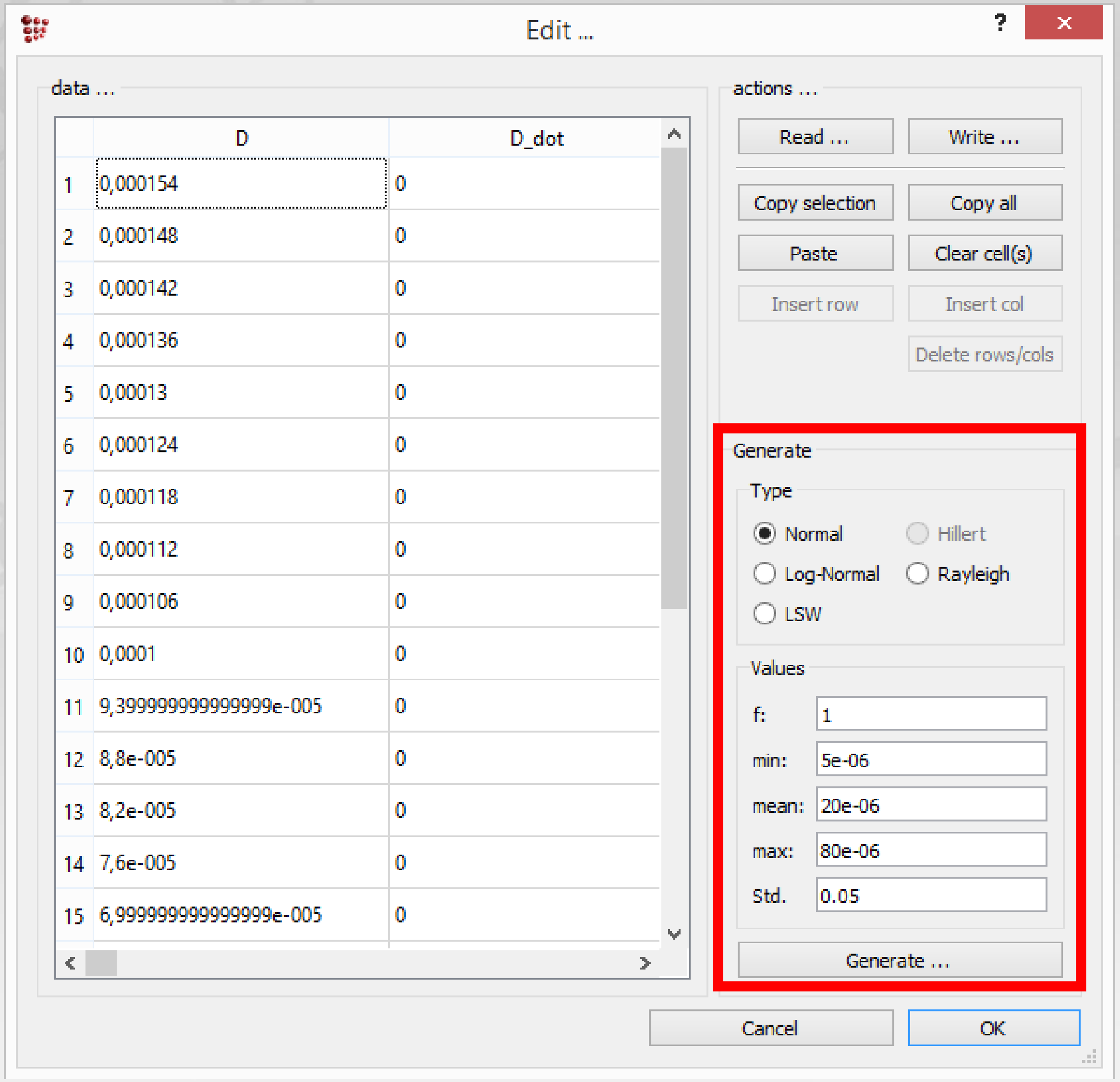
data ...

	grain_orientation_x	grain_orientation_y	grain_orientation_z	aspect_ratio_y	aspect_ratio_z	dfm_rexx	dfm_gg	gb_mob	N_dot_rexx_gb	N_dot_rexx_psn	X_N_av_dot	D_rexx	sgd_crit_drx	ro_crit_drx	fit_func
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

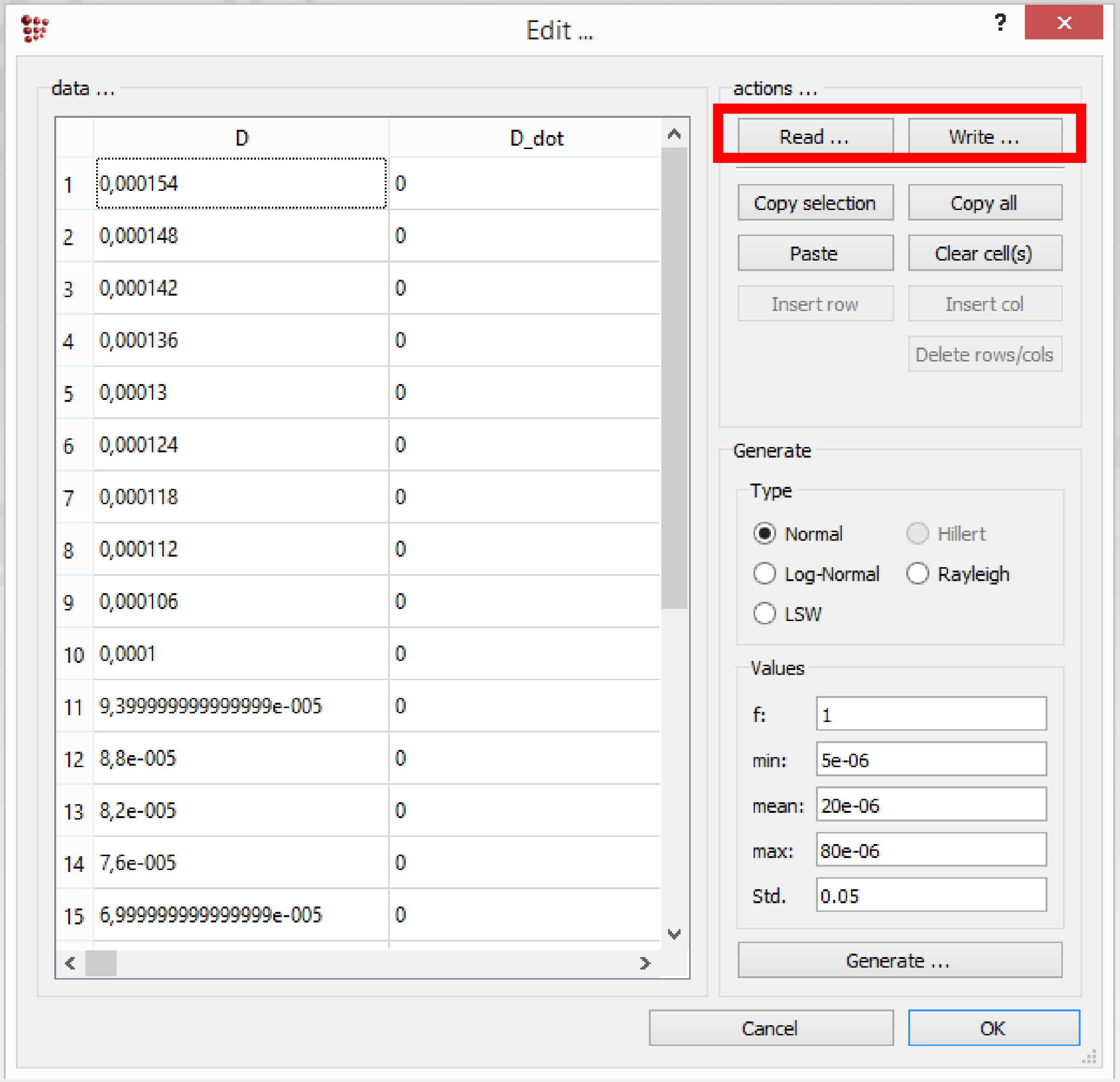
data ...

	D_mean_class	gg_wf_class	rexx_class_index	rs_h_i_factor
1	0	0	0	0,6446838...
2	0	0	0	0,2443328...

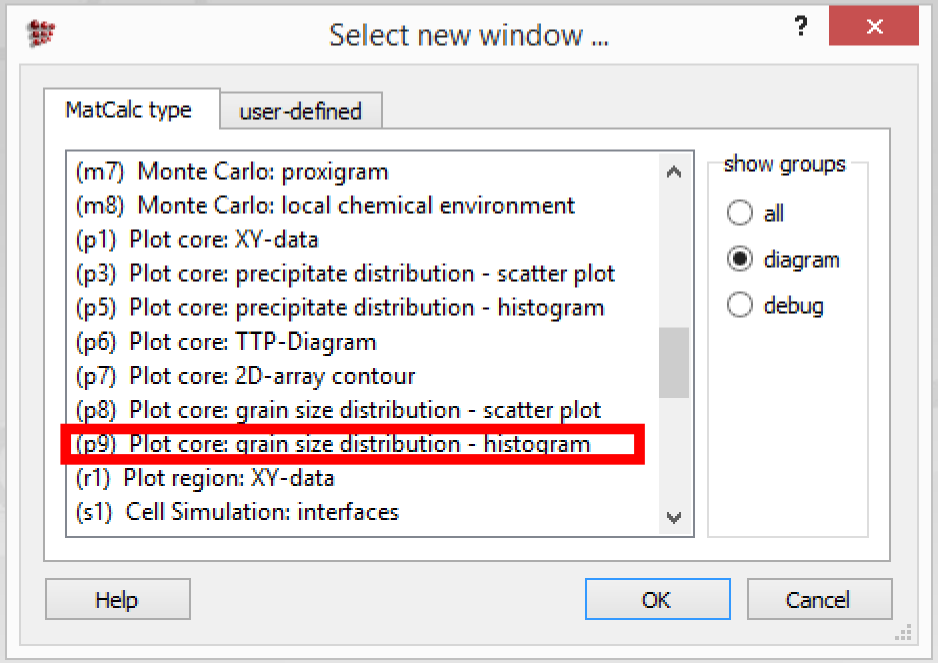
MCGM – class generation



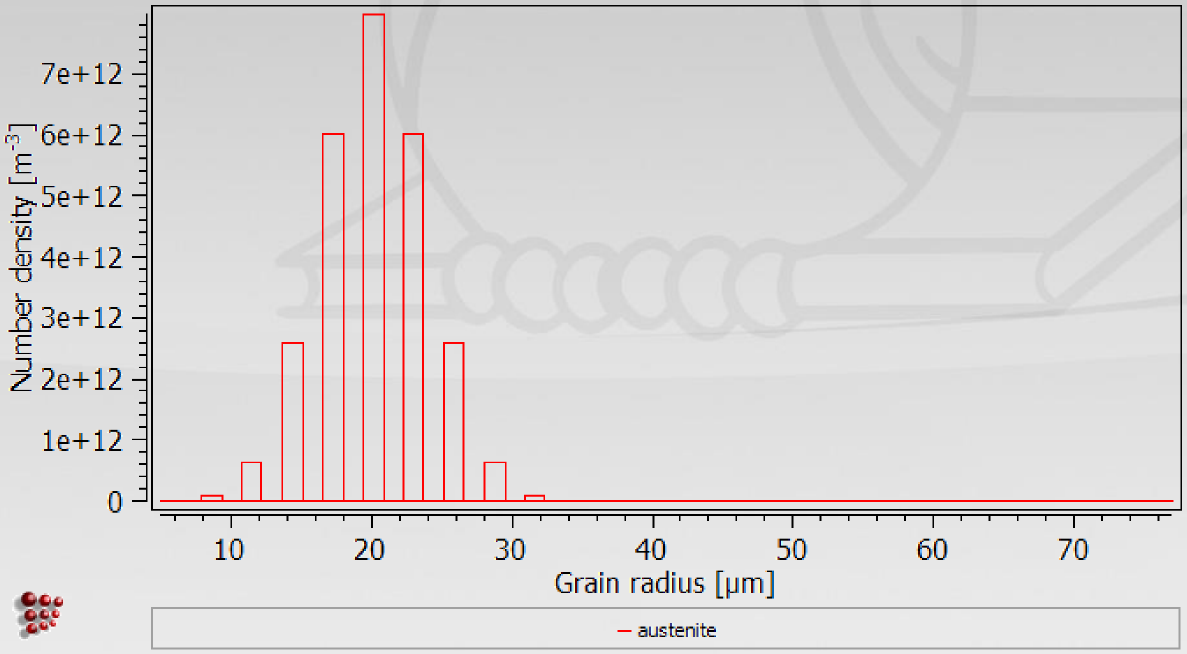
MCGM – class export/import

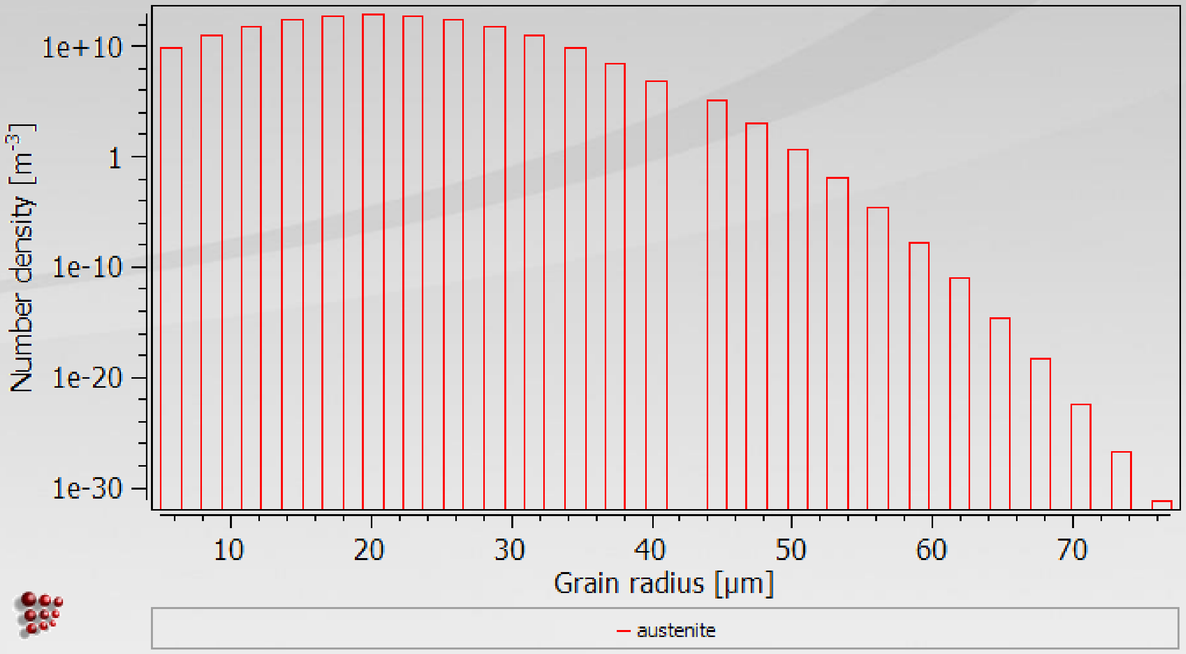


MCGM – relevant windows



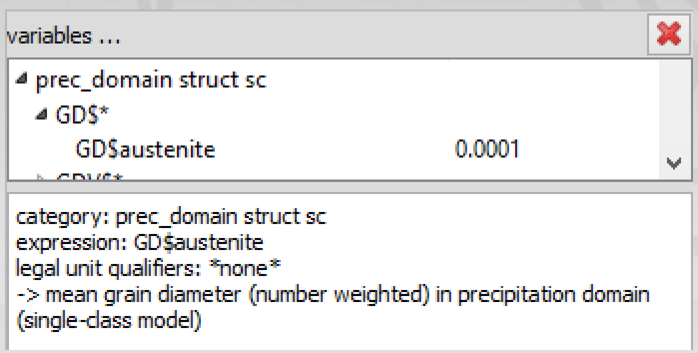
MCGM – size distribution histogram



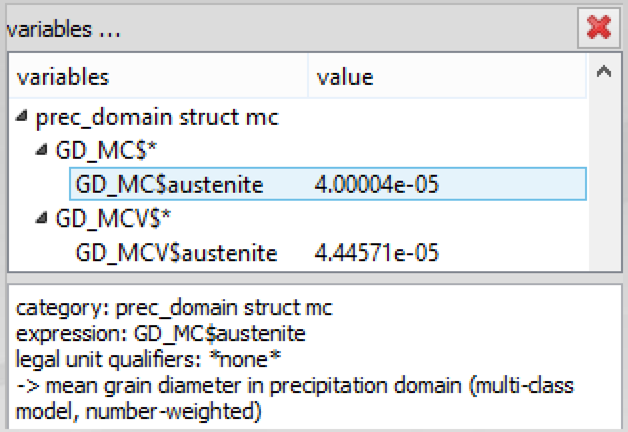


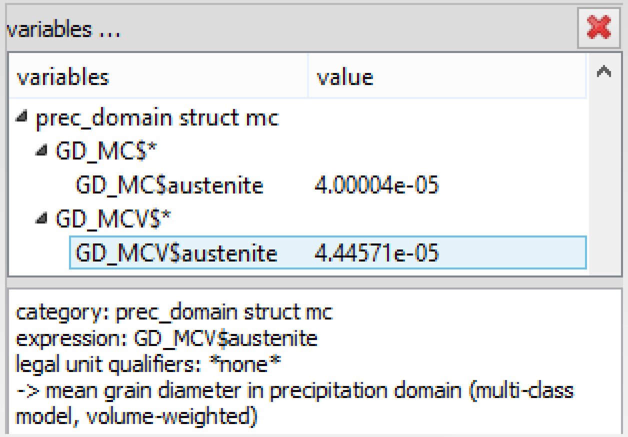
Mean grain sizes

Single class



Multi class





Grain growth kinetics model

Single class

$$\dot{D} = \frac{dD}{dt} = MP_D$$

$\dot{D}$ - Grain size growth rate

M - Grain boundary mobility

P_D - Driving force/pressure for grain growth

t - Time

Multi class

$$\dot{D}_i = \frac{dD_i}{dt} = MP_{D,i}$$

$\dot{D}_i$ - Grain size growth rate for class i

$P_{D,i}$ - Driving force/pressure for grain growth relevant to class i

Grain growth driving pressure

Single class

$$P_D = 2k_d \frac{\gamma_{HA}}{D}$$

γ_{HA} - Grain interface energy

D - Mean grain size (diameter)

k_d - Scaling factor

Multi class

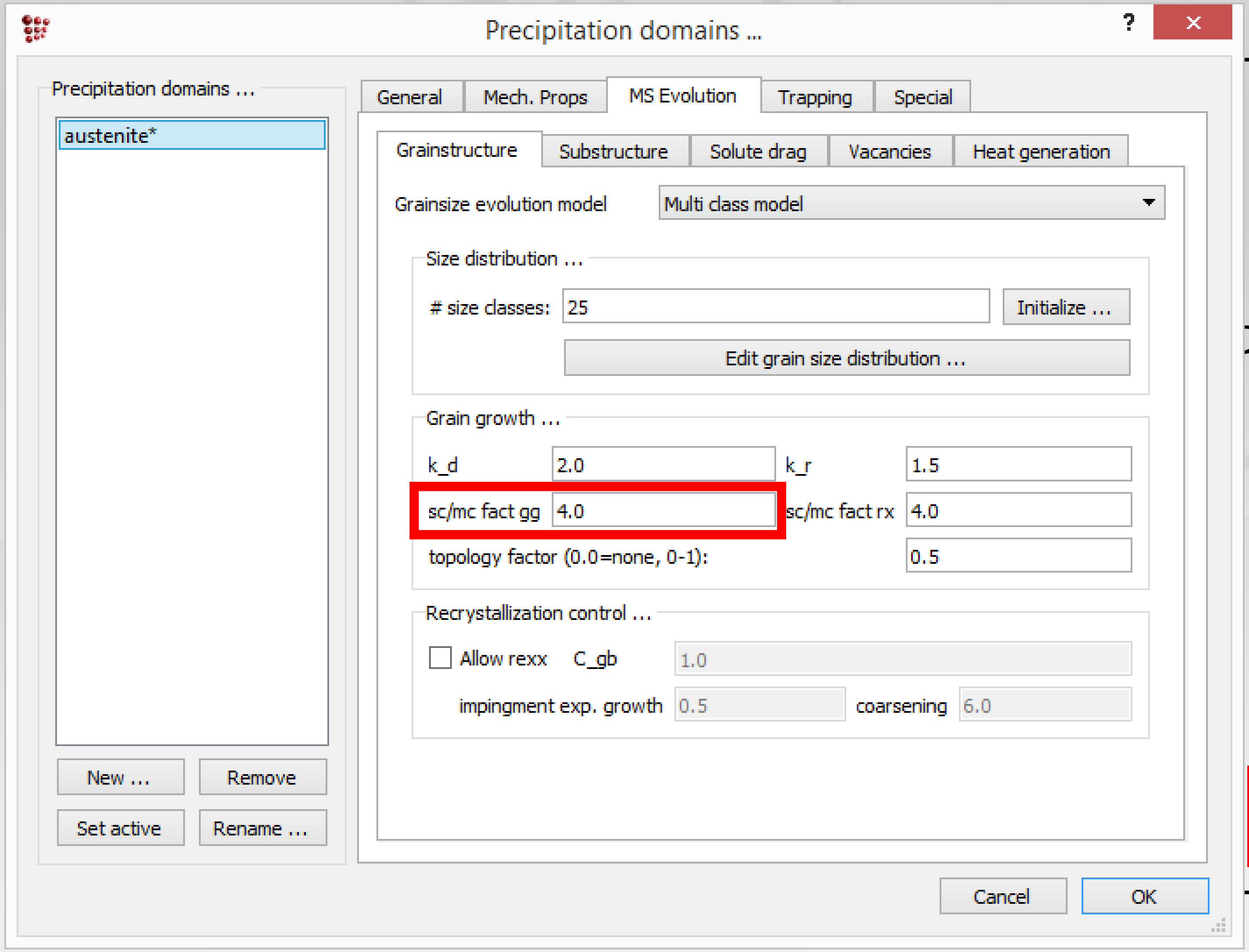
$$P_{i,D} = 2\eta_H k_d \gamma_{HA} \left(\frac{1}{D_i} - \frac{1}{D_m} \right)$$

D_i - Grain size (diameter) for class i

D_m - Mean grain size (diameter), number weighted

η_H - Scaling factor

Grain growth driving pressure



Multi class

$$P_{i,D} = 2\eta_H k_d \gamma_{HA}\left(\frac{1}{D_i} - \frac{1}{D_m}\right)$$

D_i - Grain size (diameter) for class i

D_m - Mean grain size (diameter), number weighted

$\boxed{\eta_H \text{ - Scaling factor}}$

Grain boundary mobility

$$\dot{D} = M_{eff} P_D$$

$$\frac{1}{M_{eff}} = \frac{1}{M_{prec}} + \frac{1}{M_{sd}}$$

$$M_{prec} = \begin{cases} M_p & \boxed{P_Z \geq P_D} \\ M_p \dfrac{P_Z}{P_D} + M_f \left(1 - \dfrac{P_Z}{P_D}\right) & \boxed{P_Z < P_D} \end{cases}$$

$$M_p = \eta_p M_f = \eta_p \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

M_{eff} - Effective grain boundary mobility

M_{sd} - Grain boundary mobility with solute drag

M_{prec} - Grain boundary mobility for matrix with precipitates

M_p - Grain boundary mobility for pinned interface

Grain boundary mobility

$$\dot{D} = M_{eff} P_D$$

$$\frac{1}{M_{eff}} =$$

$$M_{prec} = \begin{cases} \\ M_p \frac{\quad}{P_D} + M_f \left(1 - \frac{\quad}{P_D}\right) & \boxed{P_Z < P_D} \end{cases}$$

$$M_p = \eta_p M_f = \eta_p \eta_f \frac{\omega D_{GB} V_m}{b^2 RT}$$

Grain boundary mobility is the same for both grain size representations (single and multi class) !

M_{eff} - Effective grain

lity

lute

trix

with precipitates

M_p - Grain boundary mobility for pinned interface

Grain growth driving pressure

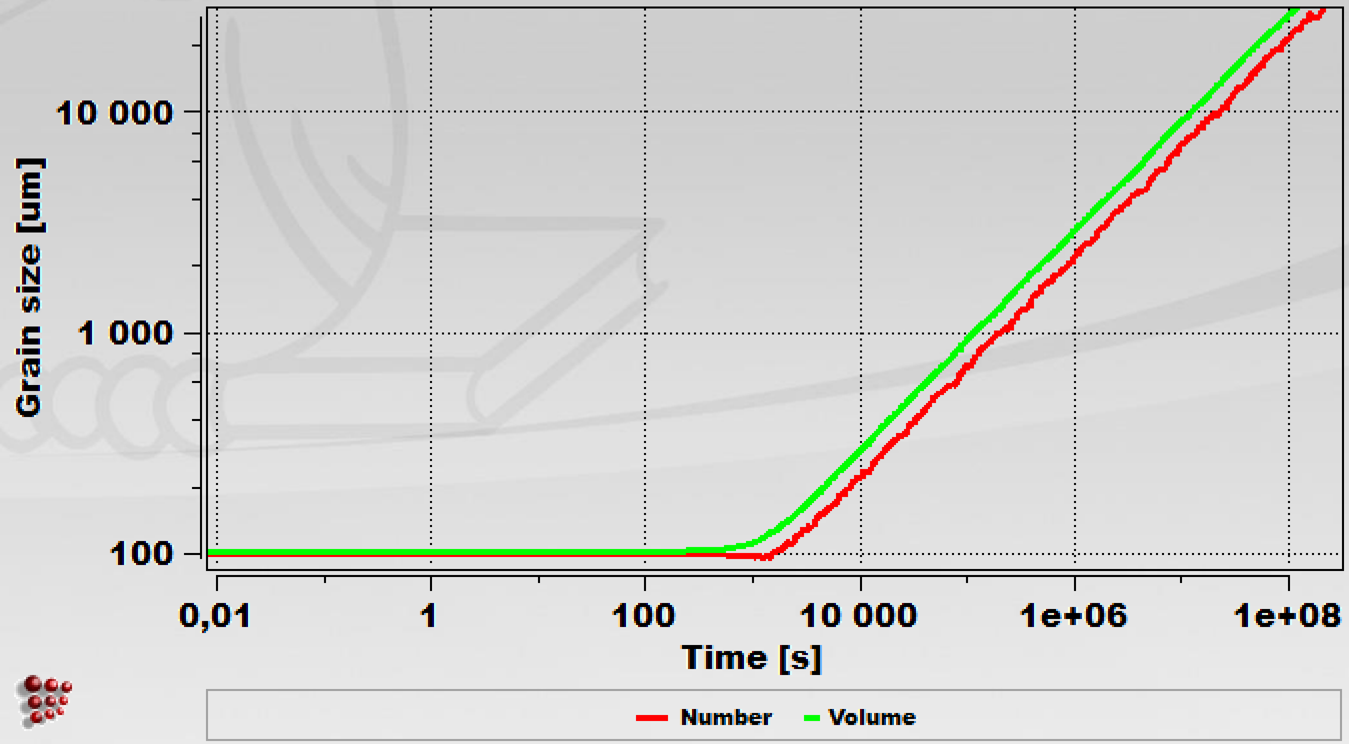
Single class

- Volume conservation by grain number adjustment

Multi class

- Volume conservation by grain size adjustment – Lagrange control volume approach

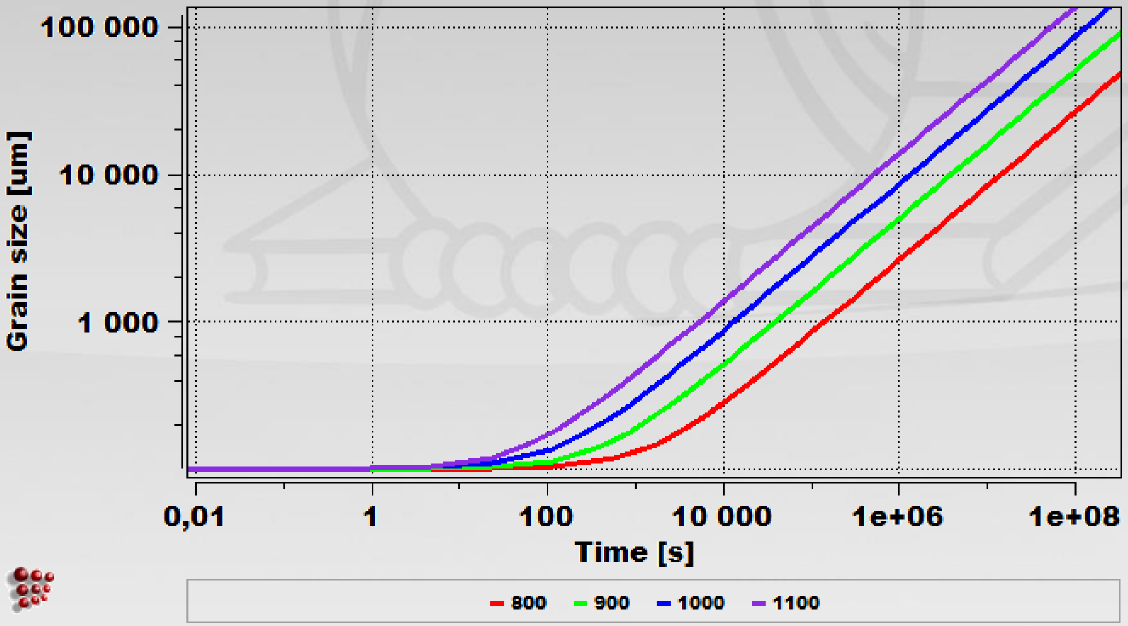
Grain growth kinetics



No obstacles

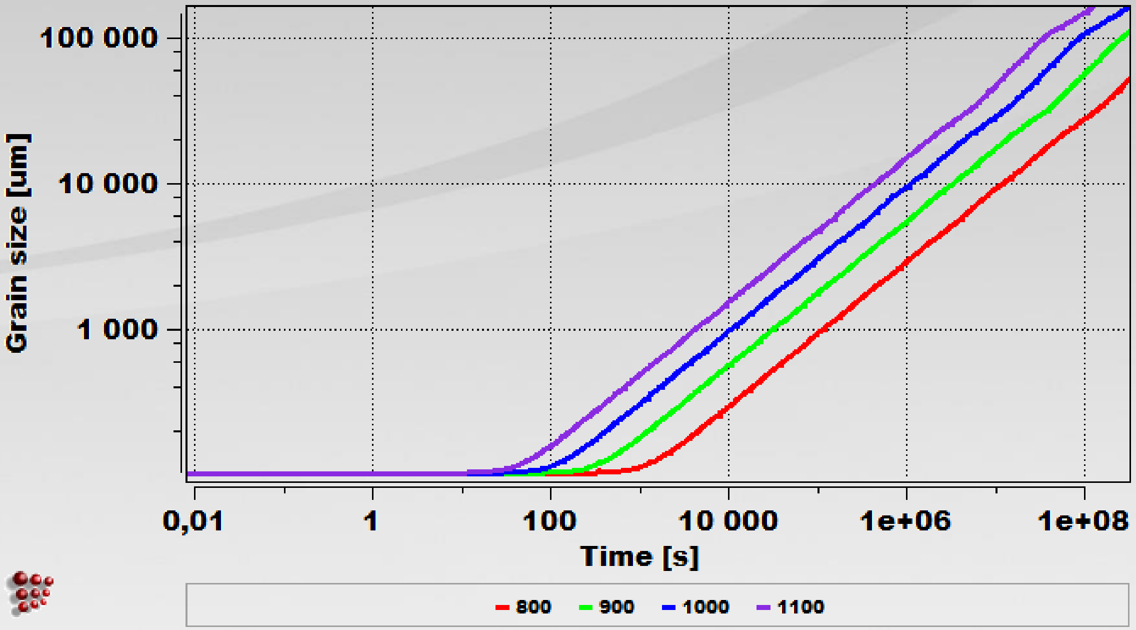
Grain growth kinetics

Single class



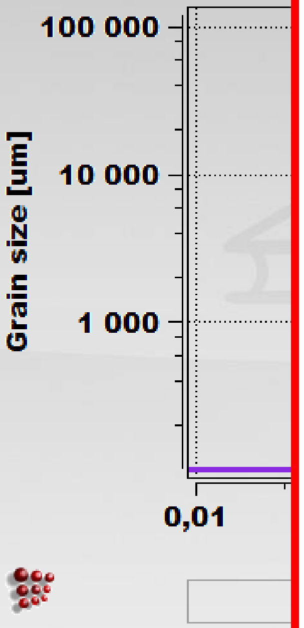
Multi class

(volume weighted)



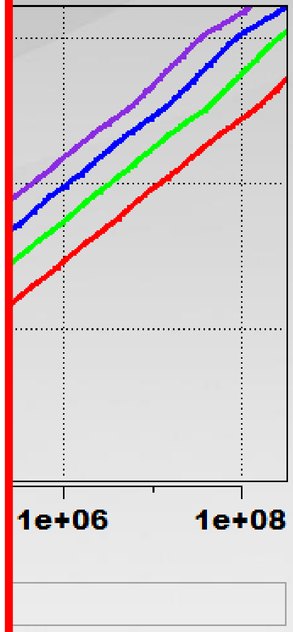
No obstacles

Grain growth kinetics



When performing multiple calculation with multi class model:

- Save a calc-state before the start of the first calculation (to save the generated grain size distribution)
- Start every calculation with the saved calc-state as the starting condition



No obstacles

Acknowledgments

- Heinrich Buken
- Yao Shan