A Combined Droplet Evaporation/Break-up Model for the Atomization of Sprays

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1 Objective

The objective of this report is to present a code, written in the popular programming language Python, which is used to model the evaporation and break-up of a continuous stream of liquid droplets within a cross-flow. This simplified approach is used to emulate the process of a spray undergoing atomization.

In section 2, the basic advection scheme for a droplet in cross-flow is presented. In section 3, the semi-empirical evaporation model, assuming constant droplet temperature, will be presented. In section 4, the Taylor Analogy Break-up (TAB) model will be presented. The TAB model simplifies the dynamics of an oscillating droplet by modelling it as a spring-mass-damper harmonic oscillator. In section 5, select results will be shown. Finally, in section ??, some final remarks will be made.

2 Droplet Advection

Droplet advection is accomplished numerically, using a second-order predictor-corrector time integration scheme. The predictor-corrector scheme has the form

$$f(t,y) = \frac{dy}{dt} \tag{1}$$

$$\tilde{y}^{n+1} = y^n + \Delta t f(t^n, y^n) \tag{2}$$

where \tilde{y}^{n+1} is the predictor step, and Δt is the time step. This step is identical to Euler time integration. The corrector step is given by

$$y^{n+1} = y^n + \frac{1}{2}\Delta t(f(t^n, y^n) + f(t^{n+1}, \tilde{y}^{n+1}))$$
(3)

In order to evaluate f(t, y), the equation for drag on a sphere, given by

$$\vec{F}_{drag} = \frac{1}{2} \rho_g |\vec{v}_{rel}|^2 c_d A_{ref} \cdot \vec{n}_{v_{rel}} \tag{4}$$

is used, where ρ_g is the air around the droplet based on T_{ref} (introduced later), \vec{v}_{rel} is the relative velocity between the droplet and the freestream, c_d is the drag coefficient which is empirically correlated, A_{ref} is the the sphere reference area, and $\vec{n}_{v_{rel}}$ is a unit vector in the direction of \vec{v}_{rel} . The drag

coefficient correlation is not given here for the sake of conciseness, but many correlations are readily available in the literature.

3 Evaporation Model

The evaporation model assumes that the droplet can be modelled from the well known " D^2 -law", which has the form

$$D^2 = D_0^2 - \lambda t \tag{5}$$

where D_0 is the original droplet diameter, and λ is the evaporation constant under quiescient conditions. For a single droplet, the rate of mass loss due to evaporation can be expressed as

$$\frac{\delta m}{\delta t} = \frac{\pi}{4} \rho_l \lambda D \tag{6}$$

where ρ_l is the liquid density. Equation (6) can be modified to account for the effects of forced convection, or cross-flow, by using the following modification:

$$\frac{\delta m'}{\delta t} = 2\pi D \left(\frac{k_g}{c_g}\right) \ln(1 + B_M) \left[1 + 0.3Re_d^{0.5} P r_g^{0.33}\right]$$
 (7)

where k_g , c_g , Re_d and Pr_g are, respectively, the thermal conductivity, the specific heat, the Reynolds number and the Prandtl number relative to the cross-flow surrounding the droplet. The mass transfer number, B_M , is computed as

$$B_M = \frac{Y_{l,s}}{1 - Y_{l,s}} \tag{8}$$

where $Y_{l,s}$ is the liquid mass fraction at the droplet surface, and must be obtained through the use of the Clausius-Clapeyron relationship. The Clausius-Clapeyron relationship is given by

$$Y_{l,s} = \frac{1}{1 + \frac{PM_g}{(P_{l,s} - 1)M_d}} \tag{9}$$

where P is the pressure surrounding the droplet, M_g is the molecular weight of the air, $P_{l,s}$ is the vapour pressure of water and M_d is the molecular weight of water. The vapour pressure of water can be found from any

number of empirical correlations, with the temperature (T_{ref}) assumed to be an average between the ambient air temperature and the temperature of the droplet. Here, the following average is used:

$$T_{ref} = T_{droplet} + \frac{T_{ambient} - T_{droplet}}{3} \tag{10}$$

With T_{ref} , the vapour pressure can be correlated. The correlation is not given here for conciseness, but they are readily available within the experimental literature.

Once the surface vapour mass fraction $(Y_{l,s})$ is known, equation (8) is used to obtain B_M , and the modified droplet evaporation constant, λ' , is computed by

$$\lambda' = \frac{8k_g \ln(1 + B_M)}{c_q \rho_l} \left[1 + 0.3Re_d^{0.5} Pr_g^{0.33} \right]$$
 (11)

where the "prime" superscript denotes a quantity which has been modified to account for advection. Equation 5 can then be used to update the droplet size at the current time step.

4 Taylor Analogy Break-up (TAB) Model

In addition to evaporation, the spray atomization model also includes a break-up model. The Taylor Analogy Break-up (TAB) model assumes the droplet can be represented by a simple spring-mass-dampter system, where the effects of surface tension are represented by the spring, the droplet mass distribution by the mass, and the effects of viscous dissipation by the damper. The model is shown graphically in figure 4.

The equation for a spring-mass-damper system is given as follows:

$$\frac{d^2y}{dt^2} + 2\zeta\omega_0\frac{dy}{dt} + \omega_0^2y = F(t) \tag{12}$$

where y is the displacement, ζ is the damping coefficient, ω_0 is the undamped natural frequency, and F(t) is a time-dependant forcing term.

For a simple droplet, the equation of motion was determined to be

$$\frac{d^2y}{dt^2} + \frac{4C_d\mu}{\rho_l d^2} \frac{dy}{dt} + \frac{8C_k\sigma}{\rho_l d^3} y = \frac{4C_f \rho_g |\vec{v}_{rel}|^2}{C_h \rho_l d^2}$$
(13)

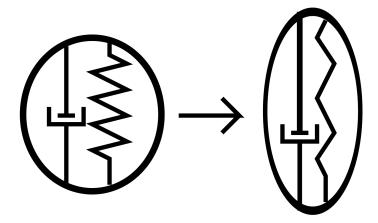


Figure 1: Droplet deformation modelled by the Taylor Analogy Break-up (TAB) model.

where μ , d, and σ are the droplet viscosity, diameter and surface tension coefficient respectively and C_d , C_k , C_f and C_b are empirically determined constants with the following values:

$$C_d = 10 \tag{14a}$$

$$C_k = 8 \tag{14b}$$

$$C_f = 2/3$$
 (gradual loading) (14c)

$$C_f = 1/3 \text{ (sudden loading)}$$
 (14d)

$$C_b = 1/2 \tag{14e}$$

The value of y is non-dimensional, and takes the form

$$y = \frac{4\Delta d_{min}}{d_0} \tag{15}$$

where d_{min} describes the deviation between the minor drop diameter and that of its original diameter, d_0 .

The solution to equation 13 has the form:

$$y(t) = We_c + e^{-t/\tau_D} \left\{ (y_0 + We_c) \cos(\omega t) + \frac{1}{\omega} \left(\frac{dy_0}{dt} + \frac{y_0 - We_c}{\tau_D} \right) \sin(\omega t) \right\}$$
(16)

where

$$\omega = \left\{ \frac{8C_k \sigma}{\rho_l d^3} - \frac{1}{\tau_D^2} \right\}^{\frac{1}{2}} \tag{17}$$

$$\tau_D = \frac{\rho_l d^2}{2C_d \mu} \tag{18}$$

and the critical Weber number, We_c , is

$$We_c = We\left(\frac{C_f}{C_k C_b}\right) \tag{19}$$

When considering a single discrete time step, and assuming that the droplet initially is not deformed nor deforming $(y_0 = \frac{dy_0}{dt} = 0)$, equation (16) and its derivative take the forms

$$y^{n+1} = We_c + e^{-\Delta t/\tau_D} \left\{ (y^n + We_c) \cos(\omega \Delta t) + \frac{1}{\omega} \left(\left(\frac{dy}{dt} \right)^n + \frac{y^n - We_c}{\tau_D} \right) \sin(\omega \Delta t) \right\}$$
(20)

$$\left(\frac{dy}{dt}\right)^{n+1} = \frac{We_c - y^{n+1}}{\tau_D} + \omega e^{-\Delta t/\tau_D} \left\{ \frac{1}{\omega} \left(\left(\frac{dy}{dt}\right)^n + \frac{y^n - We_c}{\tau_D} \right) \cos(\omega \Delta t) - (y^n - We_c) \sin(\omega \Delta t) \right\}$$
(21)

From equations (20) and (21), the distortion of each droplet may be tracked. Breakup is said to occur when y(t) > 1.

After a break-up occurs, the size of the child droplets must be determined. This is done by equating the energy of the parent droplet to the combined energy of the child droplets. The energy of the parent droplet is

$$E_{parent} = 4\pi r^2 \sigma + K \frac{\pi}{5} \rho_l r^5 \left[\left(\frac{dy}{dt} \right)^2 + \omega^2 y^2 \right]$$
 (22)

where K is the ratio of total energy in distortion and oscillation, and is set to

$$K = \frac{10}{3} \tag{23}$$

The energy of the child droplets can then be shown to be

$$E_{child} = 4\pi r^2 \sigma \frac{r}{r_{32}} + \frac{\pi}{6} \rho_l r^5 \left(\frac{dy}{dt}\right)^2 \tag{24}$$

where r_{32} is the Sauter mean radius of the droplet distribution. Setting y = 1, subbing in equation (17), and setting equations (22) and (24) equal to each other, one obtains the equation for the Sauter mean radius as

$$r_{32} = \frac{r}{1 + \frac{8Ky^2}{20} + \frac{\rho_l r^3 (dy/dt)^2}{\sigma} \left(\frac{6K - 5}{120}\right)}$$
(25)

The droplets can then be assumed to be normally distributed about r_{32} , with the number of droplets determined through mass conservation.

The velocity of the child droplets must also be computed. A normal component of velocity is added onto the droplet, which has the form

$$|\vec{v}_{normal}| = C_v C_b r \left(\frac{dy}{dt}\right) \tag{26}$$

where C_v is a constant on the order of 1.

5 Results

The following section contains results obtained from coding the evaporation and TAB droplet advection code. The code itself as been included in the appendices.

A boTAB Code - Main Module

```
1 \#!/usr/bin/env python2
2 \# -*- coding: utf-8 -*-
  " " "
4
5 boTAB
7 This_solver_uses_the_popular_TAB_model_to_simulate_the_
      atomization_of_droplets
  Author: _Adam_O'Brien
  " " "
9
10
11 from input import *
12 from math import exp, cos, sin, sqrt
13 from fluid import *
14 from evaporation import *
15 from TAB import *
16 from output import *
17 import copy as cp
18
  def main():
19
20
21
       print ""
22
       print "boTAB_|"
       print "----
23
       print "_____Compute_the_break-up_of_a_drop_in_a_
24
          uniform \( \text{cross-flow}'' \), \( \' \n'' \)
25
       # Open up a configuration file
26
27
28
       userInput = readInputFile()
29
30
       freestream = Freestream()
       initialDroplet = Droplet()
31
       dropletInlet = DropletInlet()
32
33
```

```
# Set object parameters from the input file
34
35
      setObjectParametersFromInput(userInput, freestream,
36
          initialDroplet , dropletInlet)
37
      \# Set-up the simulation parameters in accordance
38
         with the input
39
      maxTime = userInput["maxTime"]
40
      nTimeSteps = userInput["nTimeSteps"]
41
42
      # Initialize a droplet list, with one copy of the
43
         initial droplet
44
      droplets = [cp.deepcopy(initialDroplet)]
45
46
      # Initialize misc parameters
47
48
      dt = maxTime/nTimeSteps
49
50
      t = [0.]
      nChildDroplets = 0
51
52
53
      # Begin the simulation
54
      print "\nBeginning_time-stepping ..."
55
56
57
      #
58
                                              #
      #
                  Main Iteration Loop
                                              #
59
      #
60
61
      62
      for stepNo in range(1, nTimeSteps + 1):
63
64
          for droplet in droplets:
65
66
              droplet.advectPredictorCorrector(freestream
67
                 , dt)
```

```
68
           evaporate (freestream, droplets, dt)
69
           nChildDroplets += breakupTab(freestream,
70
              droplets, dt)
71
72
           dropletInlet.addDrops(initialDroplet, droplets,
           t.append(t[-1] + dt)
73
74
           if stepNo%(nTimeSteps/20) = 0:
75
76
               completionPercentage = float(stepNo)/float(
77
                  nTimeSteps) * 100.
78
79
               print "
                print "Time-stepping_completion___:_%s\%"
80
                  %(completionPercentage)
               print "Number_of_droplets_in_domain_:", len
81
                   (droplets)
                print "Simulation_time_elapsed___:_%s_
82
                  seconds "%(t[-1])
               print "Simulation_time_remaining___: _%s_
83
                   seconds" \% (maxTime - t[-1])
84
               print "Number_of_child_drops___:",
                   nChildDroplets
85
       print "\nTime-stepping complete. Finalizing output
86
87
       plotDroplets (droplets)
88
89
90 # Execute the main function
91
92 \text{ if } -\text{name} = \text{"-main}:
93
       main()
```

B boTAB Code - Fluid Module

```
2 \#/usr/bin/env python2
3 \# -*- coding: utf-8 -*-
  11 11 11
5
6 boTAB
8 This_module_contains_classes_and_function_for_the_
      modelling_of_droplets_in
9 freestream_flows
10 Author: _Adam_O'Brien
   " " "
11
12
13 from math import sqrt, pi, exp
14 import copy as cp
15 import random
16
  # Vector class for position/velocity
17
18
   class Vector(object):
19
20
       \mathbf{def} __init__(self, x, y):
21
22
            self.x = x
23
            self.y = y
24
       def __repr__(self):
25
26
            return "%s, _%s" %(self.x, self.y)
27
28
29
       \mathbf{def} --add--(self, other):
30
31
            return Vector(self.x + other.x, self.y + other.
               y)
32
       \mathbf{def} __sub__(self, other):
33
```

```
34
            return Vector(self.x - other.x, self.y - other.
35
               y)
36
37
       \mathbf{def} __mul__(self, other):
38
            return Vector(self.x*other, self.y*other)
39
40
       def mag(self):
41
            return sqrt (self.x**2 + self.y**2)
42
43
       def normalVector(self):
44
45
            return Vector (self.y, -self.x)
46
47
       def scale (self, other):
            return Vector (self.x*other, self.y*other)
48
49
       def rVector(self, other):
50
51
            return other - self
52
53
       def unitVector(self):
54
55
            return self.scale(1./self.mag())
56
57
58
   \mathbf{def} \, \det(\mathbf{u}, \mathbf{v}):
59
       return u.x*v.x + u.y*v.y
60
61
62 # Freestream class for representing the freestream flow
64 class Freestream (object):
65
       \mathbf{def}_{--}init_-(self, velocity = Vector(40., 0.),
66
           gravity = Vector(0., 0.):
67
            # constructed properties
68
69
```

```
70
            self.velocity = velocity
            self.gravity = gravity
71
72
            # default air proplerties (can be changed)
73
74
            self.mu = 18.27e-6
75
            self.Pambient = 101325.
76
            self.Tambient = 800.
77
            self.Cp = 1.0005
78
            self.k = 0.0257
79
            self.M = 28.97
80
            self.Pr = self.Cp*self.mu/self.k
81
82
83
            # Computed properties
84
            self.rho = self.Pambient/(286.9*self.Tambient)
85
86
   # Droplet class for representing droplets
87
88
   class Droplet (object):
90
        def_{-init_{-}}(self, radius = 5e-4, position = Vector)
91
           (0., 0.), velocity = Vector (0., 10.):
92
            # constructed properties
93
94
95
            self.radius = radius
            self.position = position
96
            self.velocity = velocity
97
98
            # default water properties (can be changed)
99
100
            self.rho = 998.
101
102
            self.mu = 8.94e-4
            self.sigma = 0.07262
103
            self.Tboil = 373.
104
            self.Tcrit = 647.096
105
            self.T = 400.
106
```

```
self.L = 2257.
107
             self.Cp = 4.183
108
             self.k = 0.58
109
             self.M = 18.01528
110
111
             # TAB properties
112
113
             self.y = 0.
114
             self.dydt = 0.
115
116
        \mathbf{def} __repr__(self):
117
118
119
             return "Radius: \sqrt[3]{s} \setminus n Position: \sqrt[3]{s} \setminus n Velocity: \sqrt[3]{s}"
                self.position, self.velocity)
120
121
        def diameter (self):
122
123
             return 2.*self.radius
124
125
        def volume (self):
126
127
             return (4./3.)*pi*self.radius**3
128
129
        def area (self):
130
131
132
             return pi*self.radius**2
133
        def mass(self):
134
135
             return self.volume()*self.rho
136
137
        def Pvap(self, freestream):
138
139
             Tref = (2./3.) * self.T + (1./3.) * freestream.
140
                 Tambient
141
             a1 = -7.85951783
142
```

```
a2 = 1.84408259
143
144
            a3 = -11.7866497
            a4 = 22.6807411
145
            a5 = -15.9618719
146
            a6 = 1.80122502
147
148
            tau = 1. - Tref/self.Tcrit
149
150
            pOverPc = exp((a1*tau + a2*tau**1.5 + a3*tau**3))
151
                + a4*tau**3.5 + a5*tau**4 + a6*tau**7.5)*
               self. Tcrit/self.T)
152
153
            return pOverPc*22064.
154
        def We(self , freestream):
155
156
            vRel = self.velocity.rVector(freestream.
157
               velocity)
158
            return freestream.rho*dot(vRel, vRel)*self.
159
               radius/self.sigma
160
        def Re(self, freestream):
161
162
            return freestream.rho*(freestream.velocity -
163
               self.velocity).mag()*self.diameter()/
               freestream.mu
164
        def dragCoefficient (self, freestream):
165
166
            \# This drag coefficient for a sphere is based
167
               on the correlation of
            # F.A. Morrison in "An Introduction to Fluid
168
               Mechanics"
169
            Re = self.Re(freestream)
170
171
```

```
return 24./\text{Re} + 2.6*(\text{Re}/5.)/(1. + (\text{Re}/5.))
172
               **1.52) + 0.411*(Re/263000.)**-7.94/(1. + (
               Re/263000.)**-8.) + (Re**0.8/461000.)
173
        def dragForce(self, freestream):
174
175
            Cd = self.dragCoefficient(freestream)
176
177
            vRel = freestream.velocity - self.velocity
178
179
            return vRel.unitVector()*0.5*freestream.rho*dot
180
               (vRel, vRel)*Cd*self.area()
181
182
        def acceleration (self, freestream):
183
            return self.dragForce(freestream).scale(1./self
184
                .mass()) + freestream.gravity
185
        def advectEuler(self, freestream, dt):
186
187
            a = self.acceleration(freestream)
188
189
            self.position += self.velocity*dt + a*0.5*dt**2
190
            self.velocity += a*dt
191
192
193
        def advectPredictorCorrector(self, freestream, dt):
194
            originalPosition = self.position
195
196
            a = self.acceleration(freestream)
197
            f1 = self.velocity + a*0.5*dt
198
199
            self.position += f1*dt
200
201
202
            a = self.acceleration(freestream)
            f2 = self.velocity + a*0.5*dt
203
204
```

```
205
            self.position = originalPosition + (f1 + f2)
               *0.5*dt
            self.velocity += a*dt
206
207
208
        def printAll(self):
209
            print "Radius:", self.radius
210
            print "Rho:", self.rho
211
            print "mu:", self.mu
212
            print "sigma:", self.sigma
213
            print "Boiling_Temp:", self.boilingTemp
214
            print "Latent_Heat:", self.latentHeat
215
216
            print "Specific Heat:", self.specificHeat
            print "k:", self.k
217
            print "Position:", self.position
218
            print "Velocity:", self.velocity
219
220
221
   class DropletInlet(object):
222
223
        def __init__(self, newDropletFrequency = 1000,
           inletWidth = 0.005, velocityDeviation = 0.):
224
            self.newDropletFrequency = newDropletFrequency
225
            self.inletWidth = inletWidth
226
            self.velocityDeviation = velocityDeviation
227
228
            self.timeSinceLastDroplet = 0.
229
            self.newDropletPeriod = 1./self.
               newDropletFrequency
            self.dropsAdded = 0
230
231
        def addDrops(self, initialDroplet, droplets, dt):
232
233
234
            self.timeSinceLastDroplet += dt
235
            nDropsToAdd = int(self.timeSinceLastDroplet/
236
               self.newDropletPeriod)
            self.timeSinceLastDroplet -= float (nDropsToAdd)
237
               *self.newDropletPeriod
```

```
238
            if nDropsToAdd > 0:
239
                self.dropsAdded += nDropsToAdd
240
241
            for i in range(0, nDropsToAdd):
242
243
                droplets.append(cp.deepcopy(initialDroplet)
244
245
                droplets[-1].position.x += random.uniform
                   (-0.5*self.inletWidth, 0.5*self.
                   inletWidth)
                droplets[-1].velocity.x += random.
246
                   normalvariate (0., self.velocityDeviation
                   .x)
247
                droplets[-1].velocity.y += random.
                   normalvariate (0., self.velocity Deviation
                   . y)
```

C boTAB Code - Input Module

```
2 \# -*- coding: utf-8 -*-
  " " "
5 boTAB
   This _ module _ is _ for _ simple _ file _ input _ and _ configuration
   Author: _Adam_O'Brien
   " "
9
10
  from fluid import Vector
12
  def str2num(string):
13
14
       if string.partition("/")[1] == "/":
15
16
            string = string.partition("/")
17
18
            return float (string [0]) / float (string [2])
19
20
       elif string.partition(",")[1] == ",":
21
22
23
            string = string.partition(",")
24
            return Vector(float(string[0]), float(string
25
                [2]))
26
       else:
27
28
29
            \mathbf{try}:
30
                return int(string)
31
32
            except ValueError:
33
34
```

```
return float (string)
35
36
37
  def process (inputDict, line):
38
39
       line = line.replace("\n", "")
40
       line = line.replace("", "")
41
       line = line.partition("#")
42
       line = line [0]
43
44
       if line == "":
45
           return
46
47
       line = line.partition("=")
48
49
       if not line[1] == "=":
50
           print "Warnining, potentially bad input:", line
51
52
       inputDict[line[0]] = str2num(line[2])
53
54
       return
55
56
  def readInputFile(filename = "config.in"):
57
58
       userInput = \{\}
59
60
       print "Reading_from_input_file_\"config.in\"..."
61
62
       with open(filename) as inFile:
63
64
           for line in inFile:
65
66
                process(userInput, line)
67
68
       print "The_following_input_parameters_have_been_
69
          loaded_from_\"{}\"".format(filename), "\n"
70
       for parameter in userInput:
71
```

```
72
            print parameter, "=", userInput[parameter]
73
74
        print "Finished_reading_from_input_file_\" config.in
75
76
77
        return userInput
78
   def setObjectParametersFromInput(userInput, freestream,
79
        droplet, inlet):
80
        # Freestrean properties
81
82
        freestream.rho \, = \, userInput \, [\, "freestreamRho "\, ]
83
        freestream.mu = userInput["freestreamMu"]
84
        freestream. Tambient = userInput ["freestreamTambient
85
        freestream.Cp = userInput["freestreamCp"]
86
        freestream.K = userInput["freestreamK"]
87
        freestream.velocity = userInput["freestreamVelocity
88
        freestream.gravity = userInput["freestreamGravity"]
89
        freestream.M = userInput["freestreamM"]
90
91
        # Initial droplet properties
92
93
94
        droplet.radius = userInput["dropletRadius"]
        droplet.rho = userInput["dropletRho"]
95
        droplet.mu = userInput["dropletMu"]
96
        droplet.sigma = userInput["dropletSigma"]
97
        droplet. Tboil = userInput["dropletTboil"]
98
        droplet.L = userInput["dropletL"]
99
        droplet.Cp = userInput["dropletCp"]
100
        droplet.K = userInput["dropletK"]
101
        droplet.position = userInput["dropletPosition"]
102
        droplet.velocity = userInput["dropletVelocity"]
103
        droplet.M = userInput["dropletM"]
104
105
```

D boTAB Code - Output Module

```
2 \# -*- coding: utf-8 -*-
  ;; ;; ;;
5 boTAB
  This _ module _ is _ for _ various _ plotting _ outputs
  Author: _Adam_O'Brien
  " "
9
10
11 import matplotlib.pyplot as plt
12 import matplotlib. animation as animation
13
  def plotDroplets (droplets):
14
15
       xcoords = [droplet.position.x for droplet in
16
          droplets]
       ycoords = [droplet.position.y for droplet in
17
          droplets]
       radii = [50000.*droplet.radius for droplet in
18
          droplets]
19
20
       plt.axis('equal')
       plt.grid(True)
21
       plt.xlabel('x_{-}(m)', fontsize=16)
22
       plt.ylabel('y_{-}(m)', fontsize=16)
23
24
25
       plt.scatter(xcoords, ycoords, s=radii, alpha=0.5)
26
27
       plt.show()
```

E boTAB Code - Evaporation Module

```
2 \# -*- coding: utf-8 -*-
  ;; ;; ;;
5 boTAB
  This module contains classes and function for the
      modelling_of_droplet
  evaporation_in_freestream_flows
  Author: _Adam_O'Brien
10
11
12 from math import log, sqrt, fabs, pi
  def clausiusClapeyron (freestream, droplet):
15
16
       # This function determines the water vapour mass
          fraction at the surface
       # of a droplet
17
18
       return 1./(1. + freestream.Pambient*freestream.M/((
19
          droplet.Pvap(freestream) - 1.)*droplet.M))
20
  def evaporate (freestream, droplets, dt):
21
22
       for i in range(0, len(droplets)):
23
24
           Yls = clausiusClapeyron (freestream, droplets [i
25
              ])
26
           BM = Yls/(1. - Yls)
27
28
29
           Re = droplets [i]. Re(freestream)
           Pr = freestream.Pr
30
31
```

```
32
           gamma = 8.*freestream.k*log(1. + BM)/(
              freestream . Cp*droplets [i]. rho) * (1. + 0.3*Re)
              **0.5*Pr**(1./3.)
33
           D2 = droplets [i]. diameter()**2 - gamma*dt
34
35
           if D2 > 0.:
36
37
                droplets [i]. radius = 0.5*D2**0.5
38
39
           else:
40
41
42
                droplets[i].radius = 0.
43
       # Discard any droplets that have a radius less than
44
           the tolerance, ie they
       # are completely evaporated
45
46
       droplets [:] = [droplet for droplet in droplets if
47
          not droplet.radius <= 1e-10
```

F boTAB Code - TAB Module

```
2 \# -*- coding: utf-8 -*-
4 ",","
5 boTAB
7 This_module_contains_the_functions_necessary_for_TAB_
      breakup
  Author: _Adam_O'Brien
   " " "
9
10
11 from math import exp, sin, cos, fabs
12 import numpy as np
13 import copy as cp
14 from fluid import *
15
16 # Model constants
17
18 \text{ Cb} = 0.5
19 Ck = 8.
20 \text{ Cd} = 5.
21 \text{ Cf} = 1./3.
22 \text{ Cd} = 5.
23 \text{ K} = 10./3.
24 \text{ Cv} = 1.
26 def getSMR(droplet):
27
28
       # This function computes the Sauter Mean Radius (
          SMR) of the child droplets after a break-up
29
       rOverRmean = 1. + (K/5.)*Ck*Cb**2 + droplet.rho*
30
           droplet.radius**3/droplet.sigma*Cb**2*droplet.
           dydt **2*(6.*K - 5.)/30.
31
```

```
32
       return droplet.radius/rOverRmean
33
   def breakupTab(freestream, droplets, dt):
34
35
       newDroplets = []
36
37
       for droplet in droplets:
38
39
            Wec = droplet.We(freestream)*Cf/(Ck*Cb)
40
            td = droplet.rho*droplet.diameter()**2/(2.*Cd*
41
               droplet.mu)
            omega = (8.*Ck*droplet.sigma/(droplet.rho*
42
               droplet. diameter () **3) - (1./td**2)) **0.5
43
44
            yn = droplet.y
45
            droplet.y = Wec + \exp(-dt/td) * \setminus
46
                          ((yn - Wec)*cos(omega*dt) + 1./
47
                             omega*(droplet.dydt + (yn - Wec)
                             /td)*sin(omega*dt))
48
            droplet.dydt = (Wec - droplet.y)/td + \setminus
49
                             omega*exp(-dt/td)*
50
                             (1./\text{omega}*(\text{droplet.dydt} + (\text{yn} -
51
                                Wec)/td)*cos(omega*dt) - (yn
                                - Wec) * sin (omega * dt))
52
            if droplet.y >= 1.:
53
54
                rSmr = getSMR(droplet)
55
56
57
                # Begin sampling droplets
58
                volOfNewDrops = 0.
59
60
                while True:
61
62
```

```
newRadius = np.random.normal(rSmr, 0.2*
63
                       rSmr)
64
                    if newRadius < 0.:
65
66
67
                        continue
68
                    randomNo = np.random.uniform(-1, 1)
69
70
                    newVelocity = droplet.velocity +
71
                       droplet.velocity.normalVector().
                       unitVector()*Cb*droplet.radius*
                       droplet.dydt*(randomNo/fabs(randomNo
                       ))
72
                    newDroplet = Droplet (newRadius, cp.copy
73
                       (droplet.position), cp.copy(
                       newVelocity))
74
                    newDroplets.append(newDroplet)
75
76
                    volOfNewDrops += newDroplets[-1].volume
77
                       ()
78
                    if volOfNewDrops >= droplet.volume():
79
80
81
                        break
82
       # Remove the old parent droplets
83
84
       droplets [:] = [droplet for droplet in droplets if
85
          droplet.y < 1.
86
       # Add the newly created child droplets
87
88
       for droplet in newDroplets:
89
90
           droplets.append(cp.deepcopy(droplet))
91
```

```
92
93 # Return the number of droplets created
94
95 return len(newDroplets)
```