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13. ABSTRACT (Maximum 200 words)

This is the final report for the year one effort to improve RUSTIC for Coastal, Ocean and Rolling/Rough Terrain Areas. RUSTIC, developed by ITT, is a quasi-CFD wind field modeling software intended for urban domains limited to 2 km x 2 km. This effort produced RUSTIC-CR in order to incorporate physics that are more appropriate to domains on the order of 60 km x 60 km. For larger domains, it was necessary to incorporate new terms into the governing equations as well as treat the turbulence in different ways. The effort focused on incorporating the appropriate planetary boundary layer (PBL) model for these applications. With regards to these improvements, an upgrade to the model thermodynamics was completed, physics for moist boundary layers was added, and the previous k-ω turbulence model was replaced with a second-order-closure (SOC) boundary layer model. In addition, the initial surface boundary conditions in RUSTIC-CR were improved by incorporating land use and land cover, sensible and latent heat fluxes, albedo and boundary layer height. The new product model was tested mainly in three different scenarios, Seattle, Colorado Springs, and Oklahoma City.

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Improving RUSTIC for Coastal, Ocean and Rolling/Rough Terrain Areas

Final Technical Report for Year 1

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Advanced Engineering and Sciences

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1 Introduction

This document is the final technical report for one year of work performed by ITT Corporation, Advanced Engineering & Sciences Division (AES), on the Army Research Office (ARO) sponsored tech-based project for improving RUSTIC for coastal, ocean and rolling/rough terrain areas. Several improvements and modifications have been made to the RUSTIC (Realistic Urban Spread & Transport of Intrusive Contaminants) software product to accurately include coastal and rolling/rough terrain modeling scenarios. One of the many goals of this project was for the effort to provide a highly accurate and relatively fast code that can be used to nest down to the urban environment to be used in the Urban MESO/RUSTIC GUI. The code was produced although full integration into the GUI was not. A RUSTIC-CR (Coastal and Rolling) version of RUSTIC was created during this effort to embody the large number of new physics models required for modeling wind flow in costal and rolling areas as opposed to urban areas. In addition to the nesting down techniques for urban scenarios, the RUSTIC-CR version provides superior weather models for MESO rural dispersion analysis in larger rural domains.

This effort was originally proposed as a three-year effort. This report covers the work performed during the first year. ITT was notified that tech-base priorities changed and that funding for the last two years of this project was canceled. Thus some tasks were moved into the first year, some tasks were partially completed, and other tasks cancelled. This left the RUSTIC-CR product and integration in a partial state of completion after the first year.

Prior to the development of the RUSTIC-CR, the MESO/RUSTIC suite was limited primarily by computational time and by the representative governing equations to simulations on a typical 1 km x 1 km domain with 5 m resolution. That version of MESO/RUSTIC is a coupled technique developed by ITT that simulates atmospheric dispersion and transport, in complex urban terrains, of Chemical/Biological agents. RUSTIC is the name given to the wind flow model, and MESO is the random-walk tracer-based mesoscale atmospheric transport and dispersion modeling code.

The new model development performed for this ARO contract incorporates physics that are more appropriate to larger domains on the order of 60 km x 60 km. For larger domains, it is necessary to incorporate new terms into the governing equations as well as treat the turbulence in different ways. This effort thus focused on incorporating the appropriate planetary boundary layer (PBL) model for these applications. With regards to these improvements, an upgrade to the model thermodynamics was completed, physics for moist boundary layers was added, and the previous k-ω turbulence model was replaced with a second-order-closure (SOC) boundary layer model. In addition, the initial surface boundary conditions in RUSTIC-CR were improved by incorporating land use and land cover, sensible and latent heat fluxes, albedo and boundary layer height. Upon completion of the improvements to the model, the model was tested mainly in three different scenarios, Seattle, Colorado Springs, and Oklahoma City. The results of the scenarios are shown throughout the following report sections.

Lastly, the new methodology and code were started to be incorporated into the MESO/RUSTIC GUI to facilitate ease of use for different modeling scenarios ranging from urban (1 km x 1 km) to larger (60 km x 60 km) domains. Most of the integration work was slated for years two and three of the project which was canceled.

2 Summary of Tasks

ITT modifications to RUSTIC and the MESO-RUSTIC Application Programmer's Interface (MRAPI) are documented in this summary of tasks. Table 1, lists the tasks performed to improve the models for coastal, ocean and rolling/rough terrain areas. The following subsections summarize the activities and accomplishments in performing the tasks during the period from August 2006 through August 2007.

Table 1: Tasks mapped to final report sections.

Tasks Performed	Final Report Section
Upgrade Model Thermodynamics	2.1
Add Physics for Moist Boundary Layers	2.2
Upgrading Inflow and Surface Boundary Conditions in RUSTIC	2.3
Second-Order-Closure (SOC) Boundary Layer Model	2.4
Sensible Heat Flux Model	2.5
MESO/RUSTIC API	2.6
Documentation and Verification of Model Algorithms	2.7

2.1 Upgrade Model Thermodynamics

The original RUSTIC model equations are discussed in Burrows et al. (2007). These were used as the initial starting point for this coastal and rolling tech-based development.

Model thermodynamics were upgraded to make temperature an independent variable by separating the old pressure tendency equation into a thermodynamic energy equation and a new pressure tendency equation. The new equations implemented are shown below.

For pressure tendency:

$$\frac{\partial P'}{\partial t} = -\vec{U} \bullet \vec{\nabla} P' - \bar{\rho} c^2 \left(\vec{\nabla} \bullet \vec{U} - \frac{1}{\Theta} \frac{\partial \overline{w'\theta'}}{\partial z} - (Heating - Cooling)_{moisture} \right)$$

where P' is pressure tendency, $\vec{U}$ is the velocity vector, Θ is the potential temperature, g is the gravitational constant, ρ is the density of air, C_p is the specific heat constant for a constant pressure process, $\overline{w'\theta'}$ is the second moment representing the vertical flux of temperature, and c is the speed of sound in air. The terms on the right hand side of the equation represent advection, diffusion, and pressure effects due to evaporation and condensation of moisture. In the code, the speed of sound (c), is limited to the maximum velocity occurring in the simulation.

At the surface, the equation becomes the following:

$$\frac{\partial P'}{\partial t} = -\vec{U} \bullet \vec{\nabla} P' - \bar{\rho} c^2 \left(\vec{\nabla} \bullet \vec{U} + \frac{1}{\Theta} \frac{\partial \Theta}{\partial z} \left(\frac{gz}{\Theta} \frac{Q_s}{\rho C_p} \right)^{1/3} - (Heating - Cooling)_{moisture} \right),$$

where Q_s is the sensible heat flux. Also note that a type of convection velocity scale shows up in this equation.

$$w^* = \left(\frac{gz}{\Theta} \frac{Q_s}{\rho C_p} \right)^{1/3}.$$

Then, the two newest terms accounting for evaporation and condensation in these equations are the following:

Cooling Term: $Cooling = \dfrac{L_c * EP}{C_p T(1 + 0.61r)}$

Heating Term: $Heating = \dfrac{L_c * GC}{C_p T(1 + 0.61r)}$

where T is temperature, r is the vapor mixing ratio, L_c is the latent heat of condensation/evaporation, EP is the evaporation rate, and GC is the condensation rate. EP and GC are defined by the moisture microphysics that were added to the model, and these rates have units of s^{-1}.

For the Thermodynamic Equation:

$$\frac{\partial \Theta}{\partial t} = -\vec{U} \bullet \vec{\nabla} \Theta + \left(-\frac{\partial \overline{w'\theta'}}{\partial z} + \Theta (Heating - Cooling)_{moisture} \right)$$

where $\overline{w'\theta'}$ is the second moment representing the vertical flux of temperature. The terms on the right hand side of the equation represent, advection, diffusion, and heating and cooling effects due to evaporation and condensation of moisture.

At the surface the equation becomes the following to account for sensible heat fluxes:

$$\frac{\partial \Theta}{\partial t} = -\vec{U} \bullet \vec{\nabla}\Theta + \left(w * \frac{\partial \Theta}{\partial z} + \Theta(Heating - Cooling)_{moisture} \right).$$

Note the potential temperature equation is not coupled to the pressure tendency equation in this case. In addition these equations now account for temperature and pressure changes associated with water vapor condensation and evaporation.

This process is complete and appears to perform well in initial tests. Figure 1 shows a simulation with the new thermodynamics. Warm thermals can be seen rising at scattered locations.

Upon completion this task was also incorporated into the original Urban RUSTIC without the condensation and evaporation effects.

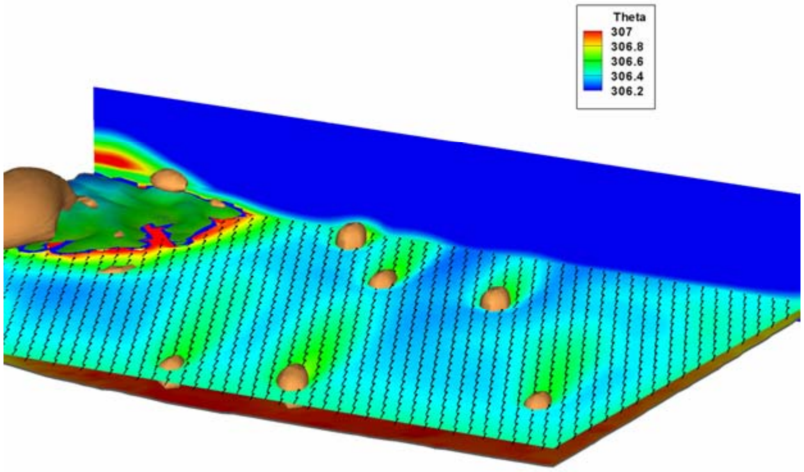


Figure 1. RUSTIC simulation with high humidity and 160º wind direction. Colors indicate potential temperature and the orange isosurfaces are where the vertical velocity is +1 m/s.

2.2 Add Physics for Moist Boundary Layers

A simple microphysical cloud and precipitation scheme developed by Kessler et al. was added to RUSTIC based on the implementation form developed by Weinstein (1970). This involved the addition of three conservation equations for water vapor, cloud water and precipitation water. The governing equations for vapor, cloud water, and precipitation are shown below.

Water vapor conservation equation:

$$\frac{\partial r}{\partial t} = -\vec{U} \bullet \vec{\nabla} r + EP - GC + SFC - r\left(\vec{\nabla} \bullet \vec{U}\right)$$

where r is the water vapor mixing ratio, $\vec{U}$ is the mean velocity vector, EP is the evaporation rate, GC is the condensation rate, and SFC is the surface moisture flux rate.

The equation describing the evaporation rate is the following:

$$EP = -kw_3(r - r_s)(\rho r_p)^{0.65},$$

where kw$_3$ = 0.001 s^{-1} is the precipitation evaporation rate constant, r$_s$ is the water saturation mixing ratio, ρ is the density of air, r$_p$ is the precipitation mixing ratio.

The water saturation mixing ratio is described by the following:

$$r_s = \frac{\varepsilon e_{s\_water}}{P - e_{s\_water}} \text{ or } r_s = \frac{\varepsilon e_{s\_ice}}{P - e_{s\_ice}}$$

where ε = 0.622 for air, e$_{s\_water}$ is the saturation vapor pressure over water, e$_{s\_ice}$ is the saturation vapor pressure over ice, and P is the ambient pressure.

The equation describing the evaporation rate is the following:

$$GC = \frac{\varepsilon e_{s\_water} W}{\rho R_D T_v^2}\left\{\frac{\frac{g}{C_p}\left(1 + \frac{L_H r_s}{R_D T_v}\right)L_H}{\left(\frac{1 + \frac{\varepsilon L_H^2 r_s}{C_p R_D T_v^2}}{R_w T}\right)} - \frac{g}{R_D}\right\},$$

where W is the mean vertical velocity, R$_D$ is the dry air gas constant, T$_v$ is the virtual temperature, L$_H$ is the latent heat of condensation or sublimation depending on the conditions, and R$_w$ is the water vapor gas constant. All other variables are as previously defined.

Finally, a surface moisture flux rate source term is given by the following when near a surface:

$$SFC = \frac{Q_L A}{\rho \forall L_c},$$

where Q$_L$ is the latent heat flux, $\forall$ is the volume of air, and A is the surface area.

Cloud water conservation equation:

$$\frac{\partial r_c}{\partial t} = -\vec{U} \bullet \vec{\nabla} r + (GC - AC - CC) - r\left(\vec{\nabla} \bullet \vec{U}\right)$$

where r_c is the cloud water mixing ratio, AC is the autoconversion rate of cloud water to precipitation, and CC is the collection rate of cloud water by precipitation (cloud water droplet scavenging by precipitation). The units of these rate terms are s^{-1}.

The autoconversion rate is given by the following:

$$AC = \frac{kw_1\left(r_c * \rho - A/1000\right)}{\rho},$$

where $kw_1 = 0.001\ s^{-1}$ is the autoconversion rate constant, and $A = 1.0\ g/m^3$ is the critical liquid water content (LWC) for autoconversion to proceed.

The cloud water collection rate is given by the following:

$$CC = kw_2 r_c (\rho r_p)^{0.875}$$

where $kw_2 = 2.1\ s^{-1}$ is the collection rate constant, and r_p is the precipitation mixing ratio.

Precipitation water conservation equation:

$$\frac{\partial r_p}{\partial t} = -\vec{U} \bullet \vec{\nabla} r + (\mathrm{FS} - \mathrm{EP} + \mathrm{AC} + \mathrm{CC}) - r\left(\vec{\nabla} \bullet \vec{U}\right)$$

where FS is the convergence of rain water due to its movement relative to air.

The convergence of rain water can be modeled as the following:

$$FS = \frac{1}{\rho}\frac{\partial(\rho r_p V_T)}{\partial z},$$

where V_T is the terminal velocity of the volume median rain drops and is positive downward. An approximation for V_T is the following:

$$V_T = kw_4 * (\rho r_p)^{1/8},$$

where $kw_4 = 12.5\ s^{-1}$ is the precipitation convergence rate constant.

Then, substitute V_T back into the original equation to obtain the following:

$$FS = \frac{kw_4}{\rho}\frac{\partial(\rho r_p)^{9/8}}{\partial z}.$$

While this microphysical model does include a crude precipitation formation algorithm, it is not likely to provide a meaningful prediction of precipitation. However, RUSTIC-CR is not intended to model precipitation processes for its applications. The main purpose of adding the moisture physics is to be able to include thermodynamic effects resulting from localized condensation and evaporation of clouds within the boundary layer. Figure 2 shows a simulation of humid conditions resulting in the formation of a cloud over the Rampart Range just northwest of Colorado Springs.

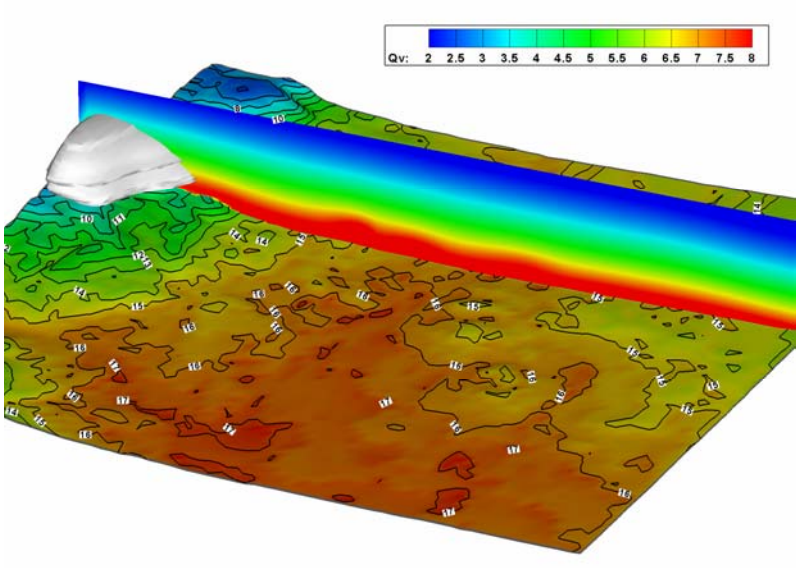


Figure 2. Same Rampart Range area of Colorado with RUSTIC-CR with color contour lines on surfaces indicating temperatures 15 m above ground. Colors on slice indicate water vapor mixing ratio. White isosurface indicates cloud water mixing ratio = 0.05 g/kg.

This task had also been left open during the development of the SOC boundary layer model to allow for any changes to the moist boundary layer algorithms as the SOC boundary layer model was developed. Once the SOC boundary layer model was running successfully, no changes to the moist boundary layer algorithms were needed.

2.3 Upgrading Inflow and Surface Boundary Conditions in RUSTIC

The first step performed under this task was to write an interface program to read the 1992 National Land Cover Dataset (NLCD) with 30 m resolution into the RUSTIC surface data structure. The NLCD contains 21 land cover classifications applied uniformly over the entire US at 1 arc sec (~30m) resolution. Figure 3 shows an example of the NLCD for Colorado Springs area. The land cover classes are listed below in Table 2.

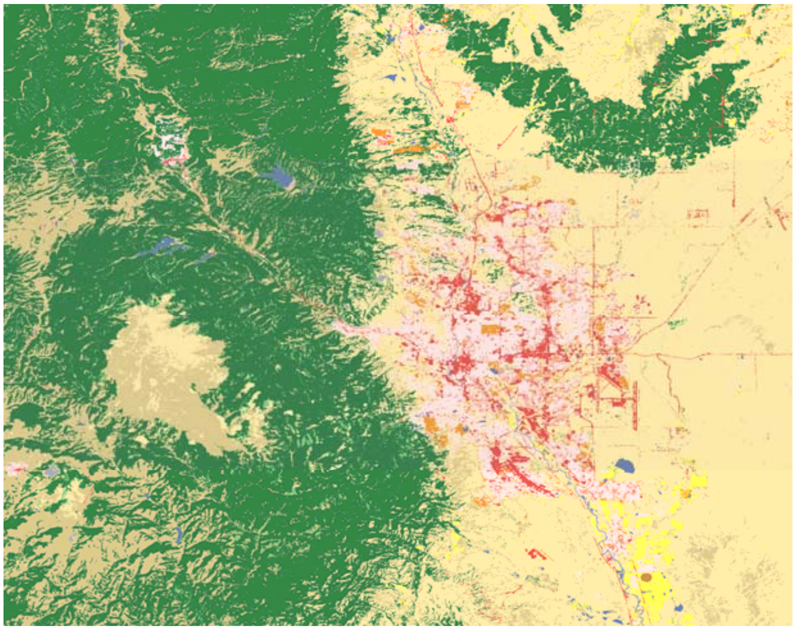


Figure 3. National Land Cover Data for the Colorado Springs area. Red and pink is for urbanized areas and roads. Green is for forested areas. Tan is for grass and brush. Yellow indicates agricultural areas and blue is for water.

The existing interface for initializing RUSTIC-CR from MM5 simulations was upgraded to include better initialization of the surface boundary conditions including sensible and latent heat fluxes, albedo and boundary layer height. For better numerical stability as RUSTIC-CR starts up, the interpolated data from MM5 is processed through an algorithm to subtract out the mean flow divergence. For initialization, RUSTIC-CR requires gridded wind fields from MM5 or an equivalent weather model. The variables that must be available in the weather model or derivable from the available variables are shown in Table 3 for the various governing equations. The surface data that must be present or derivable from MM5 or an equivalent model for the initialization of the RUSTIC-CR model is shown in Table 4. The two types of outputs from MM5 that provide the necessary variable are those that were run with the ETA-PBL model or those run with the Gayno-Seaman PBL model; both of these PBL models provide turbulent kinetic energy in the output and will currently run with the model.

Table 2. National Land Cover Dataset (NLCD) Classes.

Water	11 Open Water 12 Perennial Ice/Snow
Developed	21 Low Intensity Residential 22 High Intensity Residential 23 Commercial/Industrial/Transportation
Barren	31 Bare Rock/Sand/Clay 32 Quarries/Strip Mines/Gravel Pits 33 Transitional
Forested Upland	41 Deciduous Forest 42 Evergreen Forest 43 Mixed Forest
Shrub Land	51 Shrubland
Non-Natural Woody	61 Orchards/Vineyards/Other
Herbaceous Upland Natural/Semi-natural Vegetation	71 Grasslands/Herbaceous
Herbaceous Planted/Cultivated	81 Pasture/Hay 82 Row Crops 83 Small Grains 84 Fallow 85 Urban/Recreational Grasses
Wetlands	91 Woody Wetlands 92 Emergent Herbaceous Wetlands

Table 3. Gridded variables needed to initialize RUSTIC-CR.

Variable	Name	Source
X	x-coordinate	MM5/ACMES/Other Equivalent Model
Y	y-coordinate	MM5/ACMES/Other Equivalent Model
Z	z-coordinate	MM5/ACMES/Other Equivalent Model
U	Mean x-velocity	MM5/ACMES/Other Equivalent Model
V	Mean y-velocity	MM5/ACMES/Other Equivalent Model
W	Mean z-velocity	MM5/ACMES/Other Equivalent Model
P	Pressure	MM5/ACMES/Other Equivalent Model
Θ	Potential Temperature	MM5/ACMES/Other Equivalent Model
k	Turbulent Kinetic Energy	MM5/ACMES/Other Equivalent Model
$\overline{u'^2}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{u'v'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{u'w'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{v'^2}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{v'w'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{w'^2}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{u'\theta'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{v'\theta'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{w'\theta'}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
$\overline{\theta'^2}$	Turbulence, Second Moment	MM5/ACMES/Other Equivalent Model
r	mixing ratio, water vapor	MM5/ACMES/Other Equivalent Model
r_c	mixing ratio, cloud liquid	MM5/ACMES/Other Equivalent Model
r_p	mixing ratio, precipitation liquid	MM5/ACMES/Other Equivalent Model

Table 4. Surface variables needed to initialize RUSTIC-CR.

Variable	Name	Source
X	x-coordinate	MM5/ACMES/Other Equivalent Model
Y	y-coordinate	MM5/ACMES/Other Equivalent Model
Z	z-coordinate	MM5/ACMES/Other Equivalent Model
U_{10}	Mean x-velocity at 10 m height	MM5/ACMES/Other Equivalent Model
V_{10}	Mean y-velocity at 10 m height	MM5/ACMES/Other Equivalent Model
W_{10}	Mean z-velocity at 10 m height	MM5/ACMES/Other Equivalent Model
Surface P	Surface Pressure	MM5/ACMES/Other Equivalent Model
Surface T	Surface Temperature	MM5/ACMES/Other Equivalent Model
Surface k	Surface Turbulent Kinetic Energy	MM5/ACMES/Other Equivalent Model
Surface $\overline{\theta'^2}$	Surface turbulent second moment	MM5/ACMES/Other Equivalent Model
u*	Surface Friction Velocity	MM5/ACMES/Other Equivalent Model
Q_s	Surface Sensible Heat Flux	MM5/ACMES/Other Equivalent Model
Q_L	Surface Latent Heat Flux	MM5/ACMES/Other Equivalent Model
l	Mixing length	MM5/ACMES/Other Equivalent Model
z_i	Planetary Boundary Layer Height	MM5/ACMES/Other Equivalent Model

2.4 Second-Order-Closure (SOC) Boundary Layer Model

Instead of a true SOC scheme it was decided to use the Mellor-Yamada level-3 (1.5 order closure) turbulence scheme (Mellor and Yamada, 1974) to replace the k-ω turbulence model and which is more appropriate for larger domains. Heilman and Takle (1991) successfully used a 2-D version of this model to simulate flow over Rattlesnake Mountain in south-central Washington State.

The level-3 scheme employs prognostic equations for turbulence kinetic energy, k and the mean magnitude of the temperature fluctuations, $\overline{\theta'^2}$. Diagnostic equations are then solved for the moments: $\overline{u'u'}$, $\overline{u'v'}$, $\overline{u'w'}$, $\overline{v'v'}$, $\overline{v'w'}$, $\overline{w'w'}$, $\overline{u'\theta'}$, $\overline{v'\theta'}$, $\overline{w'\theta'}$. The

Reynold's stresses are computed directly for the momentum equation rather than the eddy diffusivity approximation. Similarly for the thermodynamic equation as previously shown the heat fluxes are computed rather than using an eddy diffusivity approximation. The main coding of this algorithm into RUSTIC-CR was accomplished in November and debugging and testing of this scheme comprised a majority of the project time.

The momentum equations for these schemes are the following:

$$\frac{\partial U}{\partial t} = -\left(U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} + W\frac{\partial U}{\partial z}\right) - \frac{1}{\rho}\frac{\partial P'}{\partial x} + \frac{\partial \overline{u'u'}}{\partial x} + \frac{\partial \overline{u'v'}}{\partial y} + \frac{\partial \overline{u'w'}}{\partial z} + fV$$

$$\frac{\partial V}{\partial t} = -\left(U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y} + W\frac{\partial V}{\partial z}\right) - \frac{1}{\rho}\frac{\partial P'}{\partial y} + \frac{\partial \overline{v'u'}}{\partial x} + \frac{\partial \overline{v'v'}}{\partial y} + \frac{\partial \overline{v'w'}}{\partial z} - fU$$

$$\frac{\partial W}{\partial t} = -\left(U\frac{\partial W}{\partial x} + V\frac{\partial W}{\partial y} + W\frac{\partial W}{\partial z}\right) - \frac{1}{\rho}\frac{\partial P'}{\partial z} + \frac{\partial \overline{w'u'}}{\partial x} + \frac{\partial \overline{w'v'}}{\partial y} + \frac{\partial \overline{w'w'}}{\partial z}$$

where U, V, W are the mean velocity components, f is the coriolis parameter, ρ is the density of air. The rest of the variables are as previously defined.

The form of the Turbulent Kinetic Energy takes the following form:

$$\frac{\partial k}{\partial t} = Advection + \mathrm{Pr}\,oduction + Diffusion + Dissipation$$

The terms for each of the right hand side components are the following:

$$Advection = -U_k\frac{\partial k}{\partial x_k}$$

$$\mathrm{Pr}\,oduction = -\overline{u_k{}'u_i{}'}\frac{\partial U_i}{\partial x_k}$$

$$Diffusion = \frac{5}{3}\frac{\partial^2\left(\lambda_1\sqrt{2}k^{3/2}\right)}{\partial x_k{}^2}$$

$$Dissipation = -\frac{\left(\sqrt{2k}\right)^3}{B_1\ell_z} = -\frac{\left(\sqrt{2k}\right)^3}{\Lambda_1}$$

$$Buoyancy = \frac{g\overline{w'\theta'}}{T} = \beta g\overline{w'\theta'} = -\beta g_k\overline{u_k'\theta'}$$

$$\lambda_1 = 0.23\,\ell_z$$

$$\ell_z = \frac{k'z}{1 + \frac{k'z}{\ell_0}}$$, mixing length Blackadar (1962) or,

$$\ell_z = k'z\,.$$

where $k^{/}$ is the von Karman constant, ℓ_0 is the mixing height above the surface, z is the height at which the mixing length is being determined, $B_1 = 15.0$, and β is the thermal expansion coefficient for air which is inversely proportional to temperature. The β assumption is a reasonable approximation and the temperature must be in degrees Kelvin.

The prognostic equation for mean magnitude of the temperature fluctuations is then the following:

$$\frac{\partial \overline{\theta'^2}}{\partial t} = Advection + \mathrm{Pr}\,oduction + Diffusion + Dissipation$$

$$Advection = -\vec{U} \bullet \vec{\nabla} k = -U_k \frac{\partial \overline{\theta'^2}}{\partial x_k}$$

$$\mathrm{Pr}\,oduction = -2\overline{u_k{}'\theta'}\frac{\partial \Theta}{\partial x_k} = -2\left(\overline{u'\theta'}\frac{\partial \Theta}{\partial x} + \overline{v'\theta'}\frac{\partial \Theta}{\partial y} + \overline{w'\theta'}\frac{\partial \Theta}{\partial z}\right)$$

$$Diffusion = \left(\frac{\partial^2\left(\overline{\theta'^2}\lambda_2\sqrt{2k}\right)}{\partial x_k{}^2}\right) =$$

$$Dissipation = -\frac{2\left(\sqrt{2k}\right)\Theta^2}{B_2\ell_z} = -\frac{2\left(\sqrt{2k}\right)\Theta^2}{\Lambda_2}$$

where $B_2 = 8.0$, and $\lambda_2 = 0.23\,\ell_z$.

The diagnostic equations are then solved for the moments: $\overline{u'u'}$, $\overline{u'v'}$, $\overline{u'w'}$, $\overline{v'v'}$, $\overline{v'w'}$, $\overline{w'w'}$, $\overline{u'\theta'}$, $\overline{v'\theta'}$, $\overline{w'\theta'}$. Assuming a boundary layer approximation, the second moments can be estimated with the following equations presented in Mellor and Yamada (1974):

$$\overline{u'w'} = \frac{-A_1\ell_z\left[\begin{array}{l}(1-3C_1)(2k)^{5/2}+6kD_f-9\beta A_2{\ell_z}^2\left\{4AC_1(2k)^{3/2}+A_2\left((2k)^{3/2}+3D_f\right)\right\}\dfrac{\partial\Theta}{\partial z}+\\ 9(\beta g)^2(2k)^{1/2}A_2{l_z}^2\left(4A_1+3A_2\right)\overline{\theta'^2}\end{array}\right]}{\left[(2k)^2+6{A_1}^2{\ell_z}^2(2k)\left|\dfrac{\partial\overline{V}}{\partial z}\right|^2+3A_1A_2{\ell_z}^2\left\{7(2k)-18A_1A_2{\ell_z}^2\left|\dfrac{\partial\overline{V}}{\partial z}\right|^2+36A_1A_2{\ell_z}^2(\beta g)\dfrac{\partial\Theta}{\partial z}\right\}(\beta g)\dfrac{\partial\Theta}{\partial z}\right]\dfrac{\partial U}{\partial z}}$$

$$\overline{v'w'} = \frac{-A_1\ell_z\left[\begin{array}{l}(1-3C_1)(2k)^{5/2}+6kD_f-9\beta A_2{\ell_z}^2\left\{4AC_1(2k)^{3/2}+A_2\left((2k)^{3/2}+3D_f\right)\right\}\dfrac{\partial\Theta}{\partial z}+\\ 9(\beta g)^2(2k)^{1/2}A_2{l_z}^2\left(4A_1+3A_2\right)\overline{\theta'^2}\end{array}\right]}{\left[(2k)^2+6{A_1}^2{\ell_z}^2(2k)\left|\dfrac{\partial\overline{V}}{\partial z}\right|^2+3A_1A_2{\ell_z}^2\left\{7(2k)-18A_1A_2{\ell_z}^2\left|\dfrac{\partial\overline{V}}{\partial z}\right|^2+36A_1A_2{\ell_z}^2(\beta g)\dfrac{\partial\Theta}{\partial z}\right\}(\beta g)\dfrac{\partial\Theta}{\partial z}\right]\dfrac{\partial V}{\partial z}}$$

$$\overline{u'v'} = -\frac{3A_1\ell_z}{(2k)^{1/2}}\left(-\overline{u'w'}\frac{\partial V}{\partial z}-\overline{v'w'}\frac{\partial U}{\partial z}\right)$$

$$\overline{w'\theta'} = -A_z\ell_z\frac{\left[\left\{\left((2k)^{3/2}+3D_f\right)-6A_1\ell_z(P_{xx}+P_{yy})\right\}\dfrac{\partial\Theta}{\partial z}-3\beta g(2k)^{1/2}\overline{\theta'^2}\right]}{\left((2k)+12A_1A_2{\ell_z}^2\beta g\dfrac{\partial\Theta}{\partial z}\right)}$$

For Total Energy > 0:

$$\overline{u'u'} = \frac{2kU^2}{\left(U^2+V^2+W^2\right)}$$

$$\overline{v'v'} = \frac{2kV^2}{\left(U^2+V^2+W^2\right)}$$

$$\overline{w'w'} = \frac{2kW^2}{\left(U^2+V^2+W^2\right)}$$

For Total Energy = 0.0

$$\overline{u'u'} = \frac{2k}{3}$$
$$\overline{v'v'} = \frac{2k}{3}$$
$$\overline{w'w'} = \frac{2k}{3}$$

where the following terms within the second moment closure equations are defined as follows:

$$D_f = \frac{4}{3} A_1 \ell_z \frac{\partial^2 (\lambda_1 (2k)^{3/2})}{\partial z^2}$$

$$\left| \frac{\partial \overline{V}}{\partial z} \right|^2 = \left(\frac{\partial U}{\partial z} \right)^2 + \left(\frac{\partial V}{\partial z} \right)^2$$

$$P_{xx} = -\overline{u'w'} \frac{\partial U}{\partial z}$$

$$P_{yy} = -\overline{v'w'} \frac{\partial V}{\partial z}$$

$$P_{xy} = -\overline{u'w'} \frac{\partial V}{\partial z}$$

$$P_{yx} = -\overline{v'w'} \frac{\partial U}{\partial z} .$$

Implementation and debugging of the code took from approximately November, 2006 to April, 2007 Further testing of the behavior of the turbulence model is needed to determine if it is indeed working correctly. A sample from a simulation made with the new model is shown in Figure 4. The figure shows a 10 km long cross section from south to north through the domain. The vertical height of the cross-section is 2200 meters. The contour lines indicate the potential temperature in K. The colors on the cross-section show the south to north component of the wind, V, in m/s. Surface colors indicate terrain elevation. These results show only a very shallow boundary layer, which is reasonable for a partly cloudy period in between rain showers. The peak wind speed corresponds to a near neutral layer between the top of the boundary layer and below a stable layer higher up.

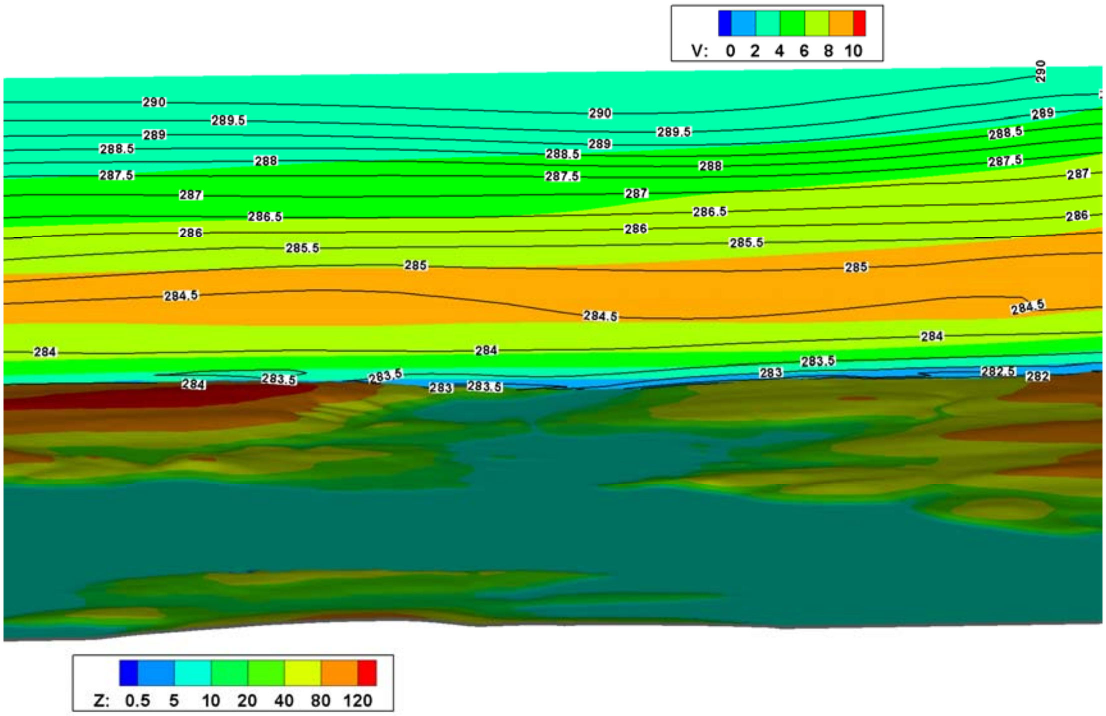


Figure 4. Results from a test run of RUSTIC-CR with the new turbulence/boundary layer model. Data is shown for a south-north cross-section through the domain about 10 km in length. The vertical height of the cross-section is 2200 meters. Contour lines are of potential temperature in Kelvin. Colors on the cross-section are of the south to north component of the wind, V, in meters per second. Surface colors indicate terrain elevation.

2.5 Sensible Heat Flux Model

A review of ITT's existing heat flux model was made to assess its accuracy for urban areas and to determine if parts of it can be used for water surfaces. In particular, the model was compared to heat flux data collected during Joint Urban 2003 in the suburbs of Oklahoma City. The heat flux data sets collected by Indiana University were downloaded from the OKC database. The files contained data taken at four suburban locations labeled BHFA, GRFA, TMFA, WHFA. The files contained 1) incoming shortwave solar, 2) net radiation, 3) latent heat, and 4) sensible heat, as well as other pertinent meteorology data. Of these, the sensible heat is the most important since it directly relates to atmospheric turbulence.

Comparison to the ITT models was made for Julian Day 190 for a couple of hours during the night and six daylight hours from 8:00 am to 6:00 pm. The primary model inputs that were extracted from the same files included 1) air temperature, 2) wind speed at a given reference height, and 3) relative humidity. For this comparison, the cloud cover input was adjusted to force agreement between the model predictions of incoming shortwave radiation and the corresponding measured values. With the exception of data in the late afternoon, the model predictions of sensible heat flux compared quite well to the data. Late in the afternoon, the model under predicted the sensible heat, probably due to heat loss from concrete and asphalt surfaces. The current model is quite simplistic for soil surfaces, but works well with surfaces covered with vegetation. This suggests the need to improve the model for water surfaces as well as for urban surfaces.

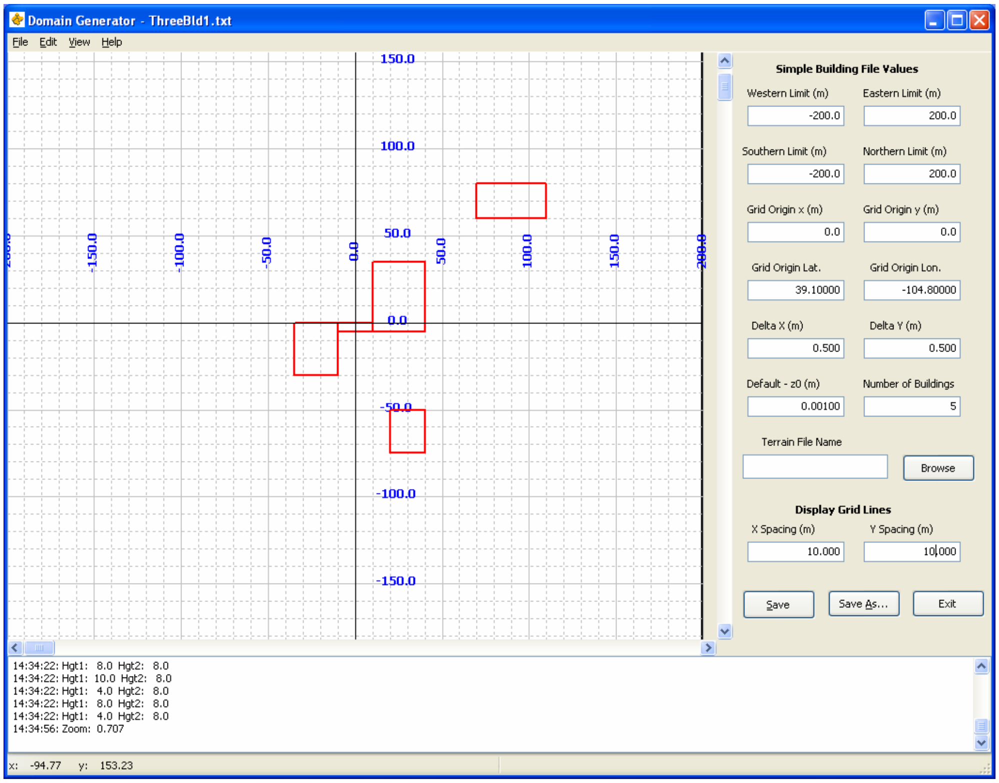
However, no additional work was done on this task beyond the initial investigation above due to the reduction in the overall length of the program. The team decided to discontinue this task for several reasons. First, this statement of work (SOW) task was scheduled for the second and third year funding which si not expected to materialize. Second, ITT in an effort to include some level of improvement decided to make an attempt to write an initial simplified version of the surface heat flux model for water surfaces in year one. But, there was soon the realization that even that version of the model could not be completed within the current funding. The current version of the model thus relies on heat flux input from initialization by MM5 or another model which produces heat flux estimates.

2.6 MESO/RUSTIC API

Enhancing RUSTIC, in this case adding coastal and rolling terrain capabilities, required corresponding changes to the MESO/RUSTIC API (MRAPI) and GUI functionality. Three main tasks were accomplished in this area with regards to adding functionality to the API/GUI:

1) Definition of Coastal and Rolling Terrains for GUI incorporation
2) Definition of initial weather (MM5 defined) for GUI incorporation
3) Setups and executions of a series of nested domains down from large coastal and rolling terrains to 1 km by 1 km complex urban domains.

The MRAPI and GUI were initially developed by ITT and enhanced in an earlier effort sponsored by the Navel Surface Warfare Center (NSWC). RUSTIC-CR specific functions were added to the MRAPI to support testing the new RUSTIC-CR functions. In addition, a few improvements were made to the GUI although most were slated to be done in the second and third years. One improvement was to modifiy the domain generator GUI that enables the user to incorporate coastal and rolling terrain features while placing features on the domain. Figure 5 shows the GUI window that the user views while placing buildings. Numerous types of digital elevation model files may be employed to define terrain.



Simple Building File Values

Western Limit (m): -200.0
Eastern Limit (m): 200.0
Southern Limit (m): -200.0
Northern Limit (m): 200.0
Grid Origin x (m): 0.0
Grid Origin y (m): 0.0
Grid Origin Lat.: 39.10000
Grid Origin Lon.: -104.80000
Delta X (m): 0.500
Delta Y (m): 0.500
Default - z0 (m): 0.00100
Number of Buildings: 5
Terrain File Name:

Display Grid Lines

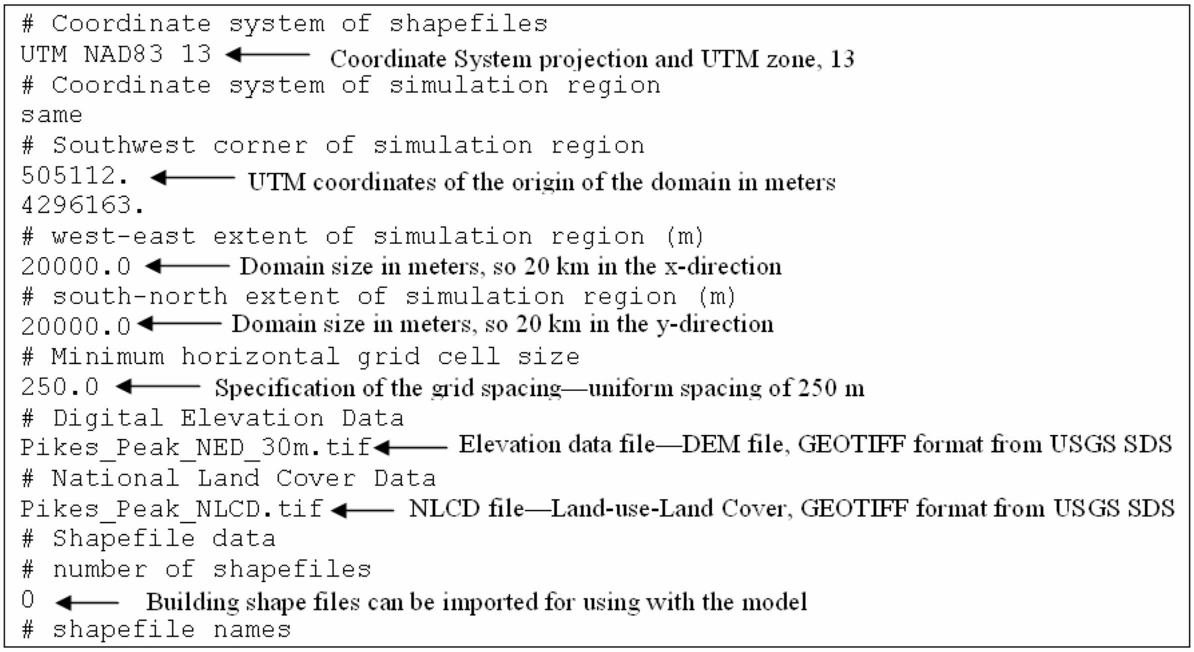
X Spacing (m): 10.000
Y Spacing (m): 10.000

```
14:34:22: Hgt1:  8.0  Hgt2:  8.0
14:34:22: Hgt1: 10.0  Hgt2:  8.0
14:34:22: Hgt1:  4.0  Hgt2:  8.0
14:34:22: Hgt1:  8.0  Hgt2:  8.0
14:34:22: Hgt1:  4.0  Hgt2:  8.0
14:34:56: Zoom: 0.707
```

x: -94.77   y: 153.23

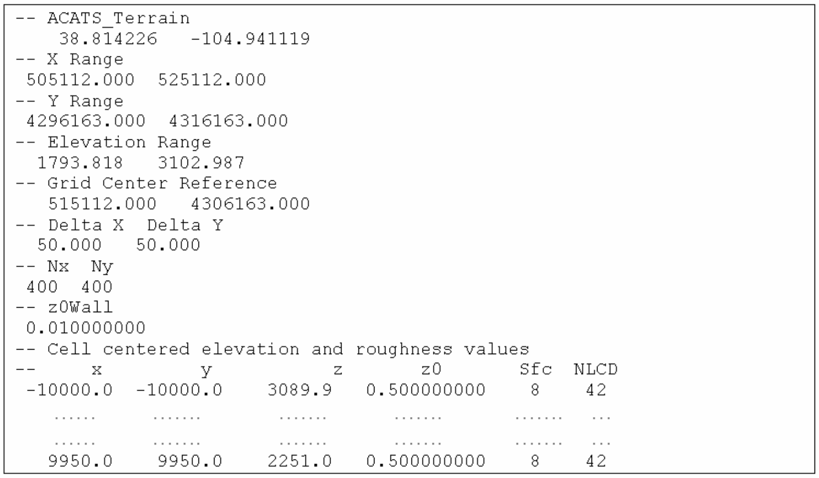
Figure 5. Domain Generator GUI.

In the new version of RUSTIC-CR, a GIS region file is used to create the terrain file. A typical region file is shown in Figure 6. The region file includes specifications for the model domain as well as the information about the files to be used for terrain and land-cover/land-use within the model. Figure 6 text is annotated with explanations for each of these features in the region file. Once the region file is created and run through the process, a terrain file is created that can be used with a grid definition (GDEF) file to create a grid. A sample terrain file created with the above region file is shown in Figure 7. The major difference between this terrain file and the previous terrain files is that this file now contains a new column for NLCD values. In addition, our grid spacing is 5 times bigger than the terrain spacing like in the Urban MESO/RUSTIC model. In fact, there is specified a 250.0 m grid spacing and the processor returned a terrain file that had 50.0 m terrain spacing. A GDEF file with desired grid spacing is now needed. A sample GDEF file that was created manually is shown in Figure 8. The grid definition requires the grid spacing used in the GIS region file be specified for the horizontal domain. In addition, the horizontal domain east-west and north-south extent must be re-specified in this file. The sample shown specifies uniform grid spacing even though it uses the linear spacing function; however, there is only one region specified with 80 divisions in each of the horizontal directions, thus the grid spacing is uniform at 250 m x 250 m for each grid cell. The vertical spacing is more involved in that 5 different vertical regions have been specified with different linear spacing in each region. As the current RUSTIC-CR code is currently written, the user could specify different regions as well. The minimum elevation in the domain can be taken from the output of the terrain file.



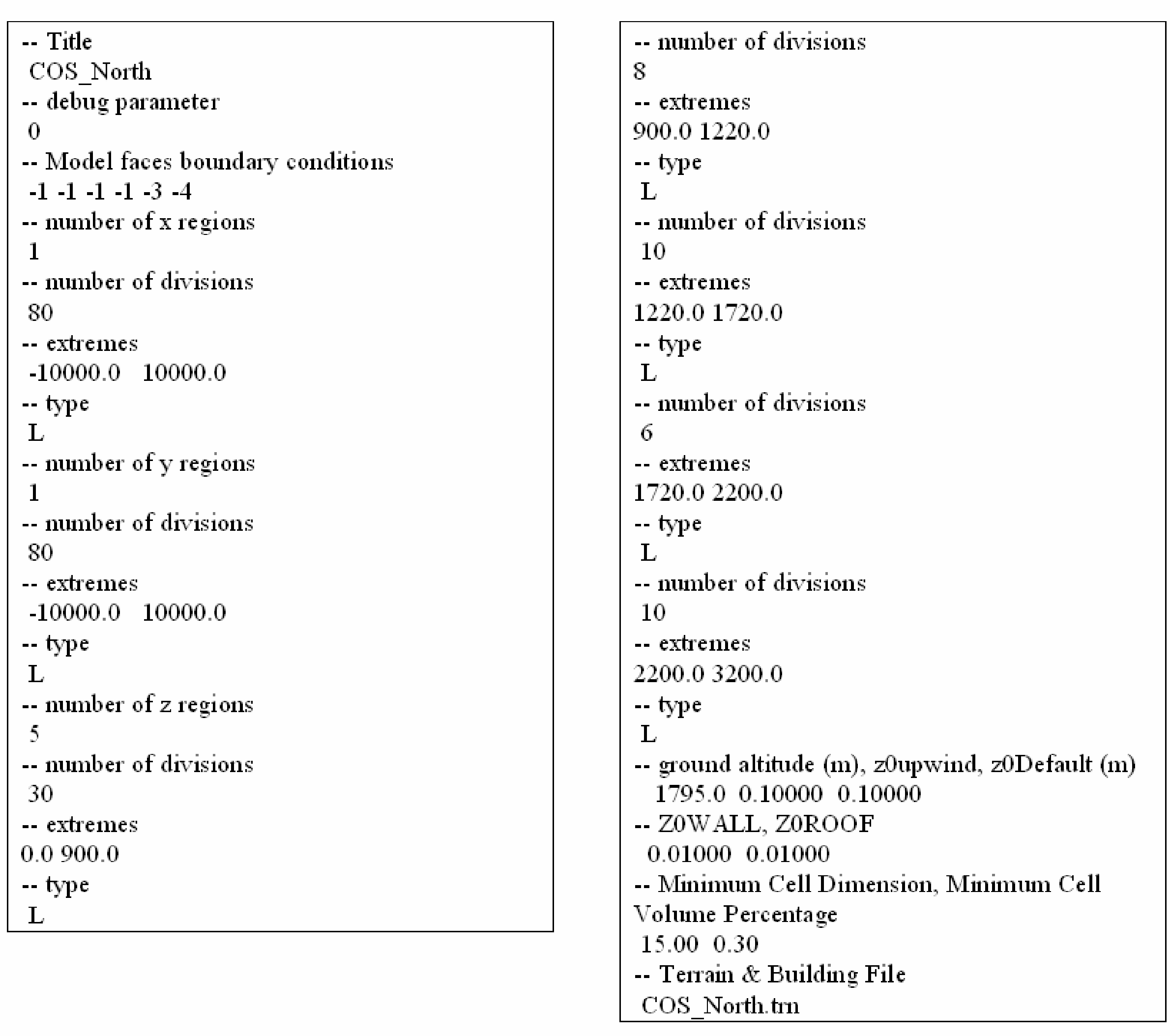
```
# Coordinate system of shapefiles
UTM NAD83 13 ←— Coordinate System projection and UTM zone, 13
# Coordinate system of simulation region
same
# Southwest corner of simulation region
505112. ←— UTM coordinates of the origin of the domain in meters
4296163.
# west-east extent of simulation region (m)
20000.0 ←— Domain size in meters, so 20 km in the x-direction
# south-north extent of simulation region (m)
20000.0←— Domain size in meters, so 20 km in the y-direction
# Minimum horizontal grid cell size
250.0 ←— Specification of the grid spacing—uniform spacing of 250 m
# Digital Elevation Data
Pikes_Peak_NED_30m.tif←— Elevation data file—DEM file, GEOTIFF format from USGS SDS
# National Land Cover Data
Pikes_Peak_NLCD.tif ←— NLCD file—Land-use-Land Cover, GEOTIFF format from USGS SDS
# Shapefile data
# number of shapefiles
0 ←— Building shape files can be imported for using with the model
# shapefile names
```

Figure 6. Sample GIS region file (*.rgn) used for Rustic-CR.



```
-- ACATS_Terrain
    38.814226   -104.941119
-- X Range
 505112.000  525112.000
-- Y Range
 4296163.000  4316163.000
-- Elevation Range
  1793.818   3102.987
-- Grid Center Reference
   515112.000   4306163.000
-- Delta X  Delta Y
  50.000   50.000
-- Nx  Ny
 400  400
-- z0Wall
 0.010000000
-- Cell centered elevation and roughness values
--      x         y           z        z0       Sfc  NLCD
 -10000.0  -10000.0    3089.9   0.500000000    8    42
    ......    .......     .......     .......     .......  ...
    ......    .......     .......     .......     .......  ...
   9950.0    9950.0    2251.0   0.500000000    8    42
```

Figure 7. Sample Terrain file (*.trn) generated with the GIS region file for Rustic-CR.



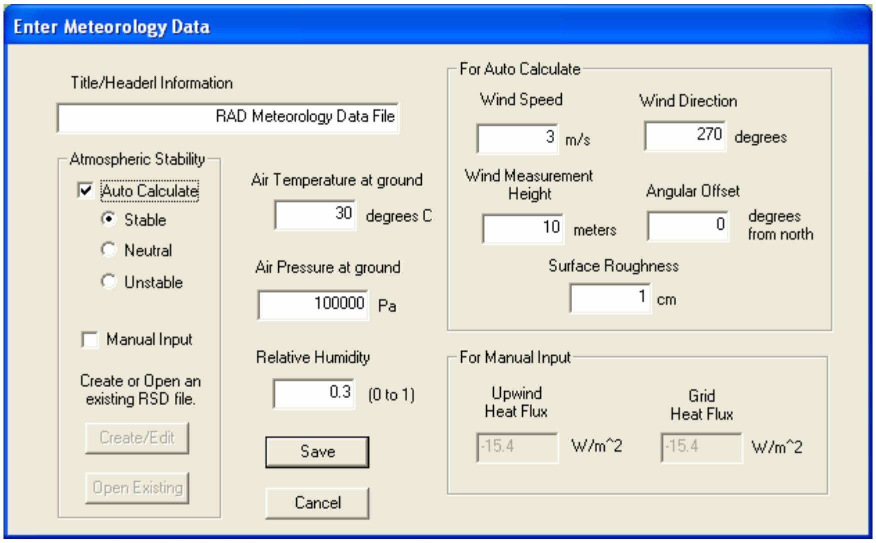
```
-- Title
 COS_North
-- debug parameter
 0
-- Model faces boundary conditions
 -1 -1 -1 -1 -3 -4
-- number of x regions
 1
-- number of divisions
 80
-- extremes
 -10000.0   10000.0
-- type
 L
-- number of y regions
 1
-- number of divisions
 80
-- extremes
 -10000.0   10000.0
-- type
 L
-- number of z regions
 5
-- number of divisions
 30
-- extremes
0.0 900.0
-- type
 L
```

```
-- number of divisions
8
-- extremes
900.0 1220.0
-- type
 L
-- number of divisions
 10
-- extremes
1220.0 1720.0
-- type
 L
-- number of divisions
 6
-- extremes
1720.0 2200.0
-- type
 L
-- number of divisions
 10
-- extremes
2200.0 3200.0
-- type
 L
-- ground altitude (m), z0upwind, z0Default (m)
   1795.0  0.10000  0.10000
-- Z0WALL, Z0ROOF
  0.01000  0.01000
-- Minimum Cell Dimension, Minimum Cell
Volume Percentage
 15.00  0.30
-- Terrain & Building File
 COS_North.trn
```

Figure 8. Sample grid definition file (*.gdef).

Once the terrain file (*.trn) and the (*.gdef) are both available, they can be used to create a grid file (*.grd). The processor creates a binary file with the grid information. The main difference between this file and previous versions of RUSTIC is that the grid file now has land-use/land-cover data. The physics engine requires that NLCD information be coded in the grid file or it will no longer work. Thus, grids created with previous versions of RUSTIC will not run in RUSTIC-CR. If the flag for NLCD is indicated as “none” in the *.rgn file, then a column of zeroes will be written to the NLCD column allowing the output files to run in RUCTIC-CR.

Another change that was slated for the GUI before funding cuts was the additional definitions of the meteorological conditions that are used to initialize RUSTIC-CR for coastal and rolling terrain models, see Figure 9. As mentioned previously, the model must be initialized by MM5 or an equivalent weather model. The two types of outputs from MM5 that provide the necessary variable are those that were run with the ETA-PBL model or those run with the Gayno-Seaman PBL model; both of these PBL models provide turbulent kinetic energy in the output. The output files from these MM5 runs should be ready to run with RUSTIC-CR. However, the MM5 output is in sigma coordinates, and thus, running the output through the INTERPB (MM5 utility) procedure to go from sigma coordinates to pressure levels seems to help with the initialization of RUSTIC-CR. The GUI was to be set-up to select the MM5 type file for use with RUSTIC-CR. This capability would allow investigators to better determine terrain and moisture effects on RUSTIC-CR modeled flow results along with transport and dispersion results in the integrated MESO/RUSTIC application.


Enter Meteorology Data

Title/Headerl Information: RAD Meteorology Data File

Atmospheric Stability
☑ Auto Calculate
● Stable
○ Neutral
○ Unstable

☐ Manual Input

Create or Open an existing RSD file.

Air Temperature at ground: 30 degrees C

Air Pressure at ground: 100000 Pa

Relative Humidity: 0.3 (0 to 1)

For Auto Calculate
Wind Speed: 3 m/s
Wind Direction: 270 degrees
Wind Measurement Height: 10 meters
Angular Offset: 0 degrees from north
Surface Roughness: 1 cm

For Manual Input
Upwind Heat Flux: -15.4 W/m^2
Grid Heat Flux: -15.4 W/m^2

Figure 9. The current dialog box of user defined meteorology options used to initialize RUSTIC. Additional parameters were slated to be added for the coastal and rolling terrain meteorology definitions.

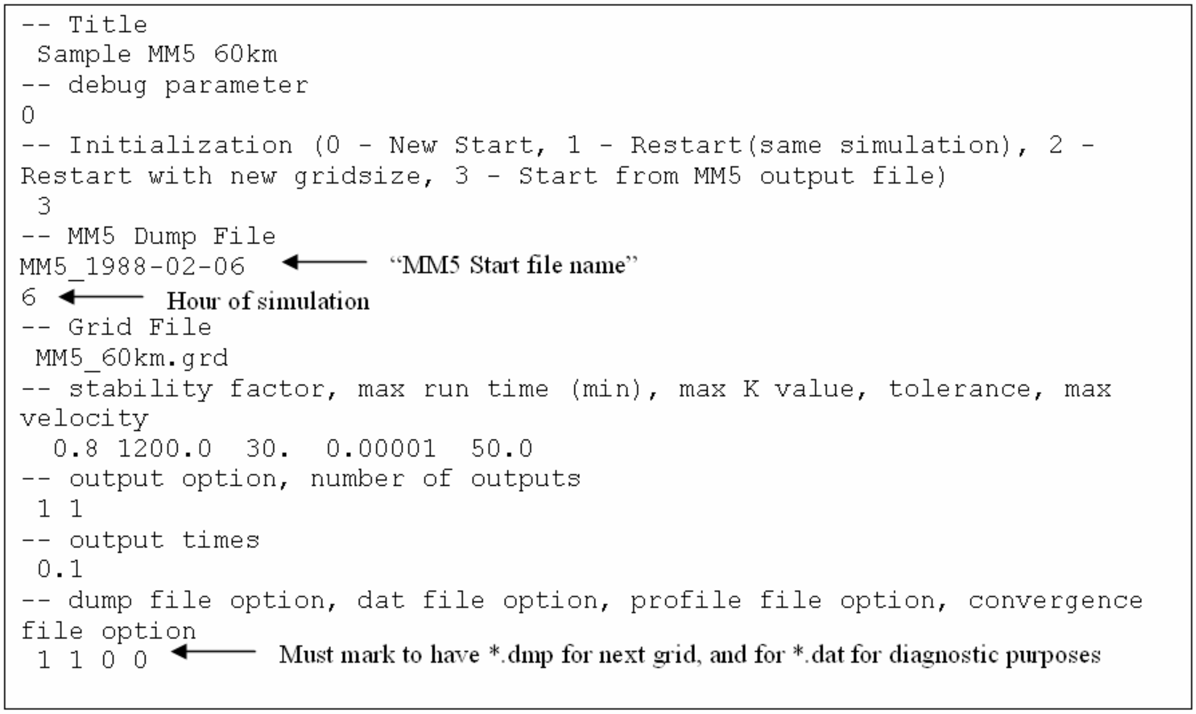
Another change that was made to the GUI is the inclusion and testing of the nested grid option to nest-down in order to provide input for MESO Rural and Urban MESO/RUSTIC simulations. For the nesting, a sample RUSTIC-CR script file is used like those shown in Figures 10 and 11. Figure 10 shows an application in which one nest is employed and then the results of RUSTIC-CR are later used for dispersion modeling with the MESO Rural model. Figure 11 shows an application in which the RUSTIC-CR model is used to nest down for use with the Urban MESO/RUSTIC models. The last nest-down is then used to initialize Urban RUSTIC. The results of Urban RUSTIC are then used with Urban MESO for dispersion analysis. A sample simulation file that the script uses is shown in Figures 12 and 13. Figure 12 shows a simulation file that initializes the first nest with MM5 data and the preprocessed *.grd file referred to earlier in the document. In addition, an output *.dmp file must be indicated; this file is used to start the second nest. Figure 13 shows a simulation file for the second nest which used a second preprocessed *.grd file appropriate for this nest (16 km grid), and the *.dmp file from the first nest. Figure 14 show the nest-down for this case.

```
2
Sample_60km_MM5_1988-02-06_06.sim
Sample_16km_MM5_1988-02-06_06.sim
```

Figure 10. RUSTIC-CR script file to create model run for use with the rural version of MESO.

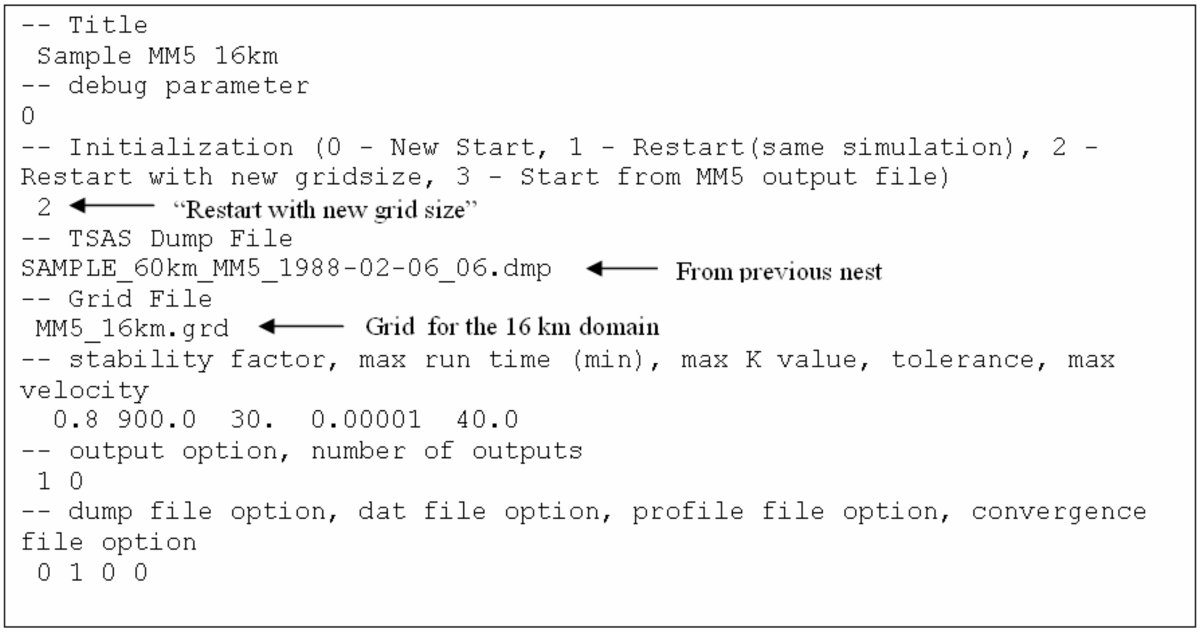
```
6
Sample_60km_MM5_1988-02-06_06.sim
Sample_16km_MM5_1988-02-06_06.sim
Sample_08km_MM5_1988-02-06_06.sim
Sample_04km_MM5_1988-02-06_06.sim
Sample_02km_MM5_1988-02-06_06.sim
```

Figure 11. RUSTIC-CR script file for nesting down to run with the urban version of MESO/RUSTIC.



```
-- Title
 Sample MM5 60km
-- debug parameter
0
-- Initialization (0 - New Start, 1 - Restart(same simulation), 2 -
Restart with new gridsize, 3 - Start from MM5 output file)
 3
-- MM5 Dump File
MM5_1988-02-06  ←  "MM5 Start file name"
6  ←  Hour of simulation
-- Grid File
 MM5_60km.grd
-- stability factor, max run time (min), max K value, tolerance, max
velocity
  0.8 1200.0  30.  0.00001  50.0
-- output option, number of outputs
 1 1
-- output times
 0.1
-- dump file option, dat file option, profile file option, convergence
file option
 1 1 0 0  ←  Must mark to have *.dmp for next grid, and for *.dat for diagnostic purposes
```

Figure 12. RUSTIC-CR simulation file for initializing the RUSTIC-CR run with MM5 data for the first 60 km domain.



```
-- Title
 Sample MM5 16km
-- debug parameter
0
-- Initialization (0 - New Start, 1 - Restart(same simulation), 2 -
Restart with new gridsize, 3 - Start from MM5 output file)
 2  ←  "Restart with new grid size"
-- TSAS Dump File
SAMPLE_60km_MM5_1988-02-06_06.dmp  ←  From previous nest
-- Grid File
 MM5_16km.grd  ←  Grid  for the 16 km domain
-- stability factor, max run time (min), max K value, tolerance, max
velocity
  0.8 900.0  30.  0.00001  40.0
-- output option, number of outputs
 1 0
-- dump file option, dat file option, profile file option, convergence
file option
 0 1 0 0
```

Figure 13. RUSTIC-CR simulation file for nesting-down to 16 km.

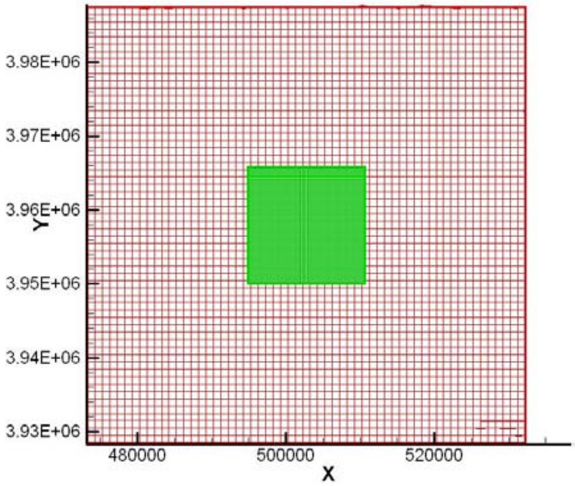


Figure 14. The RUSTIC-CR domain nest-down from 60km to 16 km.

2.7 Documentation and Verification of Model Algorithms

A test was devised to investigate the behavior of the new coastal and rolling boundary layer model under a variety of conditions of topography and atmospheric stability.

Simulations were executed for unstable conditions with little terrain, Oklahoma City (OKC), for very unstable conditions with topography and deep convection, Colorado Springs (COS), and moderately unstable to stable with a mixture of land and water surfaces, Seattle (SEA).

The vertical profiles of wind speed, turbulence kinetic energy (TKE) and potential temperature, Theta, for the OKC simulation are shown in Figure 15. The profiles are for a location near the center of the grid. The surface heat flux at this location was 341 W m^{-2} and the boundary layer depth was approximately 1200 m. The profiles vary smoothly with height as is expected for a site with even terrain overall.

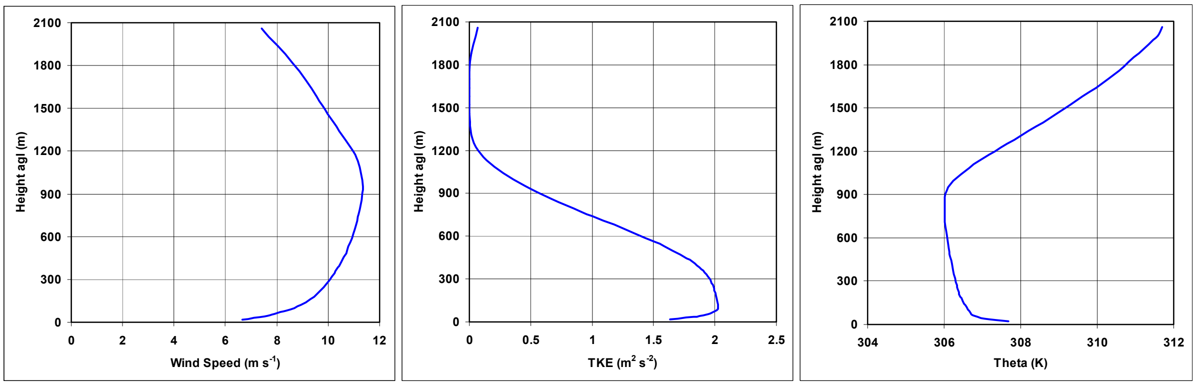


Figure 15. Vertical profiles of wind speed, TKE and Theta for a simulation for OKC on 9 July 2003 1800 UTC.

Vertical profiles of the same variables are shown in Figure 16 for COS. In this case the profiles are for a low elevation (1855 m) location about 6 kilometers from the mountain front and for a location near the top of Rampart Ridge (2734 m). At both locations the atmosphere was unstable. The sensible heat flux at the low elevation site was 229 W m^{-2} and at the high elevation site, 535 W m^{-2}. In both cases the top of the boundary layer is above the top of the grid. The MM5 simulation used for initialization contained some deep convective clouds in the area. As would be expected the site with the higher sensible heat flux develops more TKE and a higher potential temperature. The wind speed profiles are quite different as are expected due to the large variations in topography.

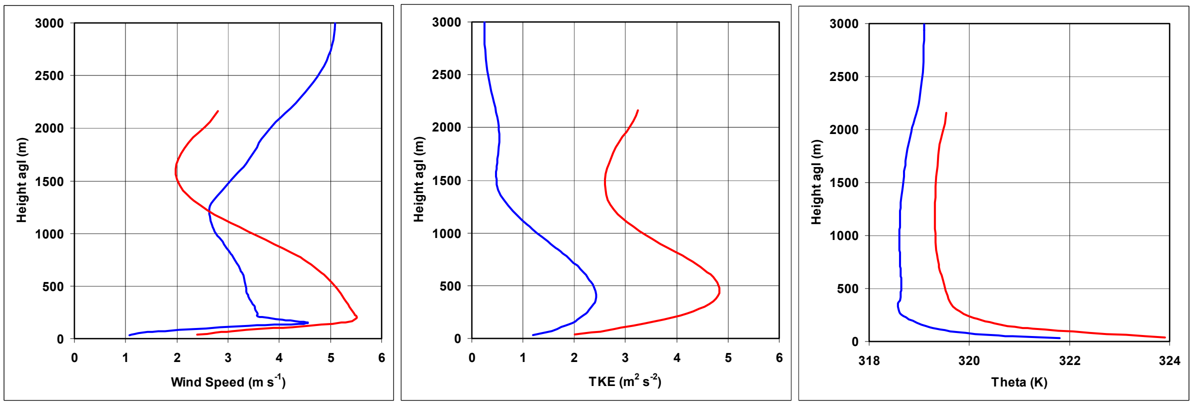


Figure 16. Vertical profiles of wind speed, TKE and Theta for a simulation for COS on 26 May 2006 1900 UTC. The blue line is for the low elevation location (1855 m) and the red line is for the higher elevation site (2734m).

The results of the third simulation are shown in Figure 17 for SEA. In this case one location is over Puget Sound and the other over land. Over the water the sensible heat flux was -20 W m^{-2}, because the water was cooler than the air. This resulted in a potential temperature profile where Theta was increasing with height at all levels. Corresponding to this there was little production of TKE at that site. Over the land the sensible heat flux was 296 W m^{-2}, in a location receiving sunshine. At this location vertical profiles of wind speed, TKE and potential temperature developed closely resembling the OKC profiles as expected.

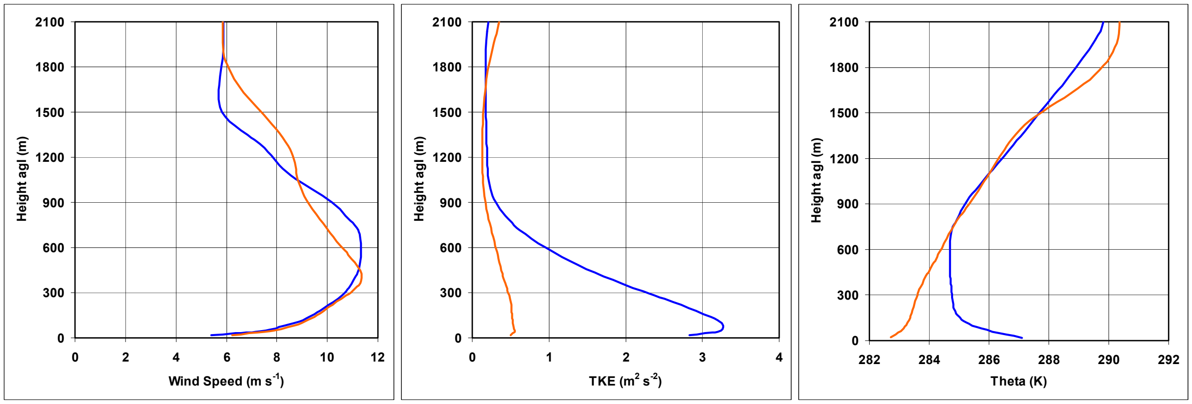


Figure 17. Vertical profiles of wind speed, TKE and Theta for a simulation for SEA on 26 May 2006 1900 UTC. The blue line is for the site over land and the red line is for the site over the Puget Sound.

Another test consisted of a four level MM5 simulation for May 26, 2006. The fourth level nest covered a 39 km x 39 km area centered on Colorado Springs and had a horizontal resolution of 750 meters as shown in Figure 18.

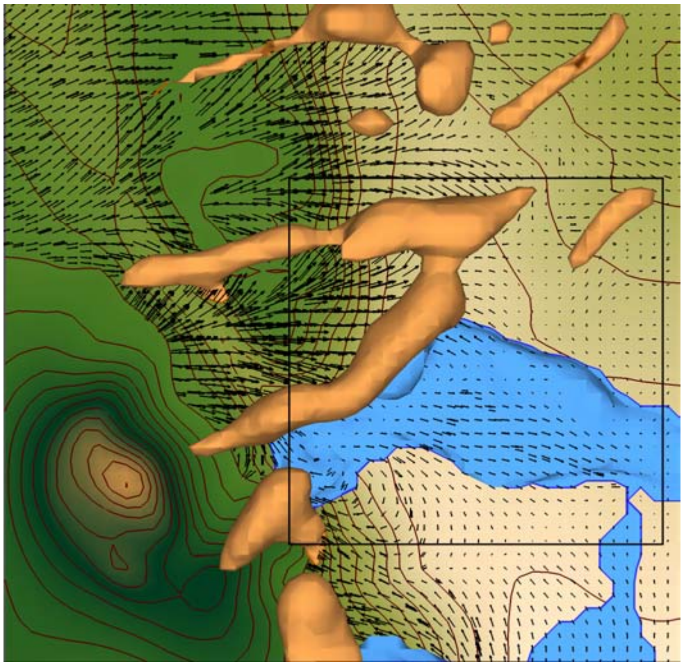


Figure 18. MM5 simulation for May 26, 2006 1700 UTC. Arrows are wind vectors at 2250 m above sea level. Orange isosurfaces are where vertical wind velocity = 1 m/s. Blue isosurface is where water vapor mixing ratio is 3 g/kg. Contour lines are surface elevation at 100 meter intervals. Grid resolution is 750 meters. Black square is the 20 km x 20 km area covered by the RUSTIC-CR simulation shown in Figure 19.

The forth level MM5 results were used to initialize RUSTIC-CR with its execution results shown in Figure 19. At this point the model upgrades are working well. Further testing and developments as part of this contract were put on hold due to the cut in funding.

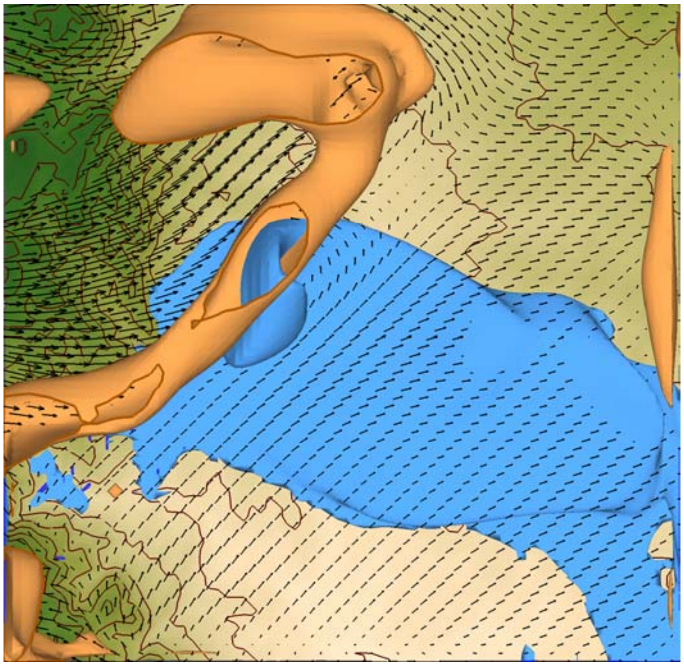


Figure 19. RUSTIC-CR simulation for May 26, 2006 1710 UTC initialized from a MM5 simulation. Wind vectors and isosurfaces are the same as in Figure 18. Holes in isosurfaces indicate that the surface extends to the top of the grid. Grid resolution is 250 meters horizontally and 30 to 100 meters in the vertical.

3 Summary

This report serves as the final report documentation for year one tasks performed in enhancing RUSTIC for coastal and rolling terrain producing the RUSTIC-CR software product. This effort was originally proposed as a three-year effort, but ITT was notified that tech-base priorities changed and funding for the last two years of this project was canceled. This caused some second and third year tasks to be moved into the first year, with some tasks partially completed, and other tasks cancelled. Much work was performed developing the RUSTIC-CR product and the product produces results, but it was left in partial state of completion after this first year effort.

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