Requirements on Wildfire-Atmosphere Modeling

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CO_2

Introduction

To simulate the interrelation between the atmosphere and wildfires as well as the fire spread, it is necessary to have a meteorological pre-processor like RAMS (Pielke, 2002) or a new development. In addition, we need modules to predict

- the oxidation of chemical species (flame chemistry),
- the release of energy generated by the combustion process,
- the pyrolysis of the wooden fuel especially by radiant heating,
- the transport of heat, water vapor, and liquid water within the soil and its impact on regions of permafrost,
- the emission of biomass burning being the source of primary pollutants (e.g., CO, CO_2, CH_4, H_2, NMHC, PAH, NO, N_2O, COS, particulate matter), and
- the chemical reactions among primary pollutants and normal atmospheric constituents in the turbulent smoke plume to form secondary pollutants that may react with primary as well as secondary pollutants and/or photo-dissociate by solar radiation to generate, for instance, free radicals.

Theoretical Background

Balance equation of reactive trace constituents

- Macroscopic system:

$$\frac{\partial(\rho\,\chi_i)}{\partial t} + \nabla\cdot\left(\rho\,\mathbf{v}\,\chi_i + \mathbf{J}_i\right) = \sigma_i\,, \qquad \chi_i = \frac{\rho_i}{\rho}$$

- Turbulent system:

Hesselberg’s averaging calculus (1926):

$$\varphi = \hat{\varphi} + \varphi'' \qquad \text{with} \qquad \hat{\varphi} = \frac{\overline{\rho\,\varphi}}{\overline{\rho}} \qquad \text{and} \qquad \overline{\rho\,\varphi''} = 0$$

$$\frac{\partial(\overline{\rho}\,\hat{\chi}_i)}{\partial t} + \nabla\cdot\left(\overline{\rho}\,\hat{\mathbf{v}}\,\hat{\chi}_i + \overline{\rho\,\mathbf{v}''\chi_i''} + \overline{\mathbf{J}}_i\right) = \overline{\sigma}_i$$

Segregation effects (Kramm & Meixner, 2000)

$$\overline{\sigma_i} = f_i\left(\overline{\rho_1},\ldots,\overline{\rho_N}\right) + f_i\left(\rho_1',\ldots,\rho_N'\right)$$

$$f_i\left(\overline{\rho_1},\ldots,\overline{\rho_N}\right) = \sum_{j=1}^{N} \overline{\rho}\,\hat{k}_{ij}\,\hat{\chi}_j + \sum_{\substack{m=1\\ n\geq m}}^{N} \hat{C}_{imn}\,\overline{\rho}\,\hat{\chi}_m\,\hat{\chi}_n$$

$$f_i\left(\rho_1',\ldots,\rho_N'\right) = \sum_{j=1}^{N} \overline{\rho\, k_{ij}''\chi_j''} + \sum_{\substack{m=1\\ n\geq m}}^{N} \Big(\hat{C}_{imn}\,\overline{\rho\,\chi_m''\chi_n''}$$

$$+ \overline{\rho\, C_{imn}''\chi_m''}\,\hat{\chi}_n + \overline{\rho\, C_{imn}''\chi_n''}\,\hat{\chi}_m$$

$$+ \overline{\rho\, C_{imn}''\chi_m''\chi_n''}\Big)$$

$$C_{imn} = \rho\, k_{imn}$$

$$f_i(\rho_1',\ldots,\rho_N') \cong \sum_{\substack{m=1 \\ n\geq m}}^{N} \hat{C}_{imn}\, \overline{\rho\, \chi_m''\, \chi_n''}$$

$$\overline{\sigma}_i \cong \sum_{j=1}^{N} \overline{\rho}\, \hat{k}_{ij}\, \hat{\chi}_j + \sum_{\substack{m=1 \\ n\geq m}}^{N} \hat{C}_{imn}\, \overline{\rho}\, \hat{\chi}_m\, \hat{\chi}_n \left(1 + I_{s,mn}\right)$$

$$I_{s,mn} = \frac{\overline{\rho\, \chi_m''\, \chi_n''}}{\overline{\rho}\, \hat{\chi}_m\, \hat{\chi}_n}$$

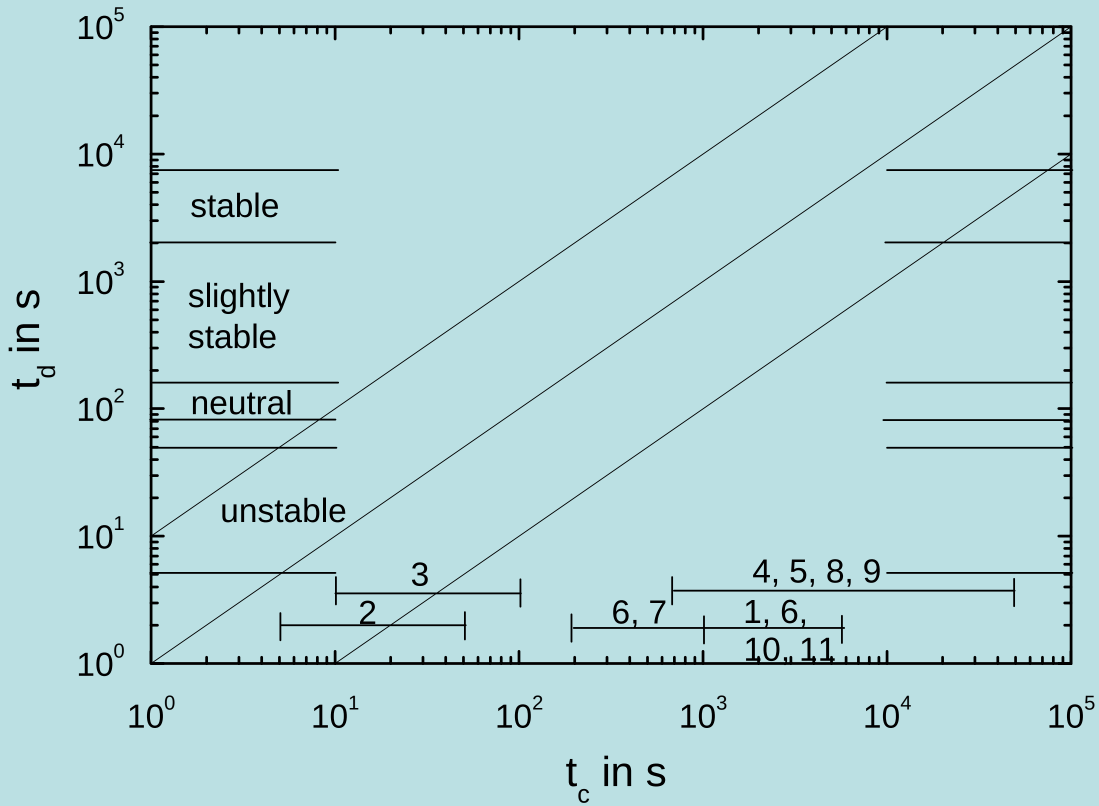
Intensity of segregation

$$-1 \leq I_{s,m,n} \leq 0$$

- Requires, at least, second-order-closure modeling

Damköhler number

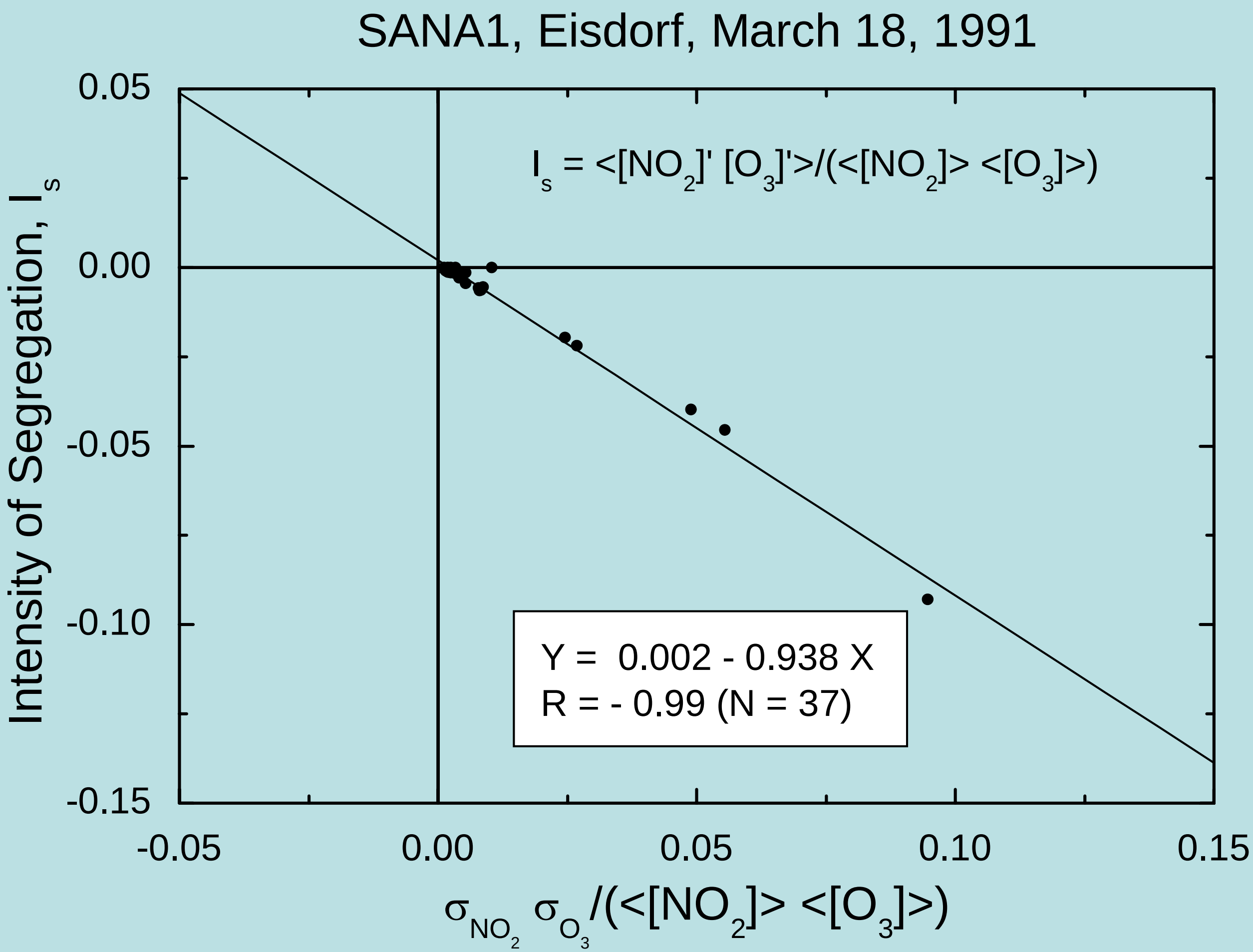
$$N_D = \frac{t_d}{t_c}$$



1. $HO_2 + HO_2 \rightarrow H_2O_2$
2. $HNO_3 + NH_3 \rightarrow NH_4NO_3$
3. $O_3 + NO \rightarrow NO_2 + O_2$
4. O_3 + Isoprenes → Products (P)
5. O_3 + Monoterpenes → P
6. NO_3 + Monoterpenes → P
7. NO_3 + Isoprenes → P
8. OH + Isoprenes → P
9. OH + Monoterpenes → P
10. O_3 + Olefins → P
11. $O_3 + NO_2 \rightarrow NO_3 + O_2$

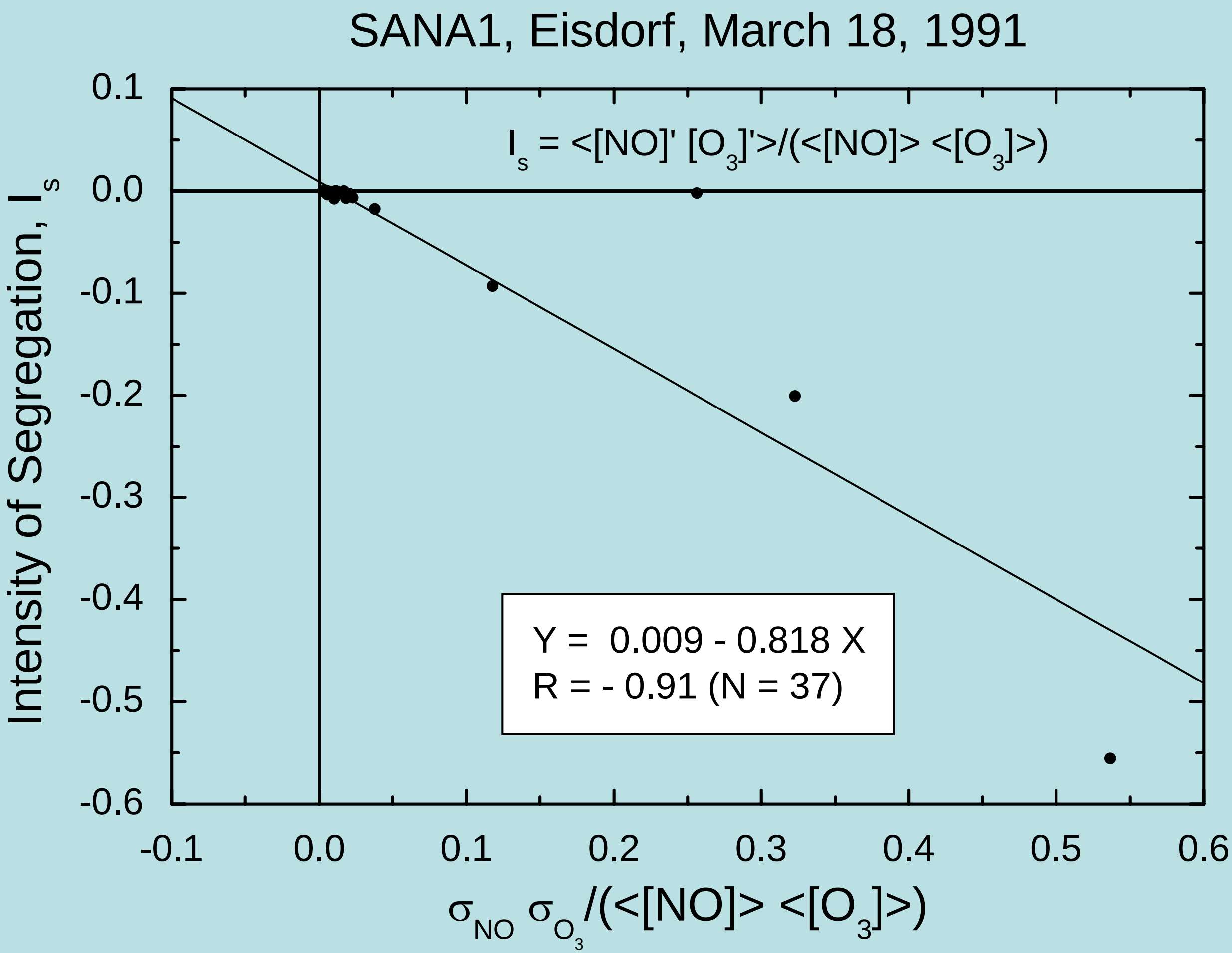
Source: Kramm & Dlugi (1994)

Intensity of segregation



Source: Kramm & Meixner (2000)

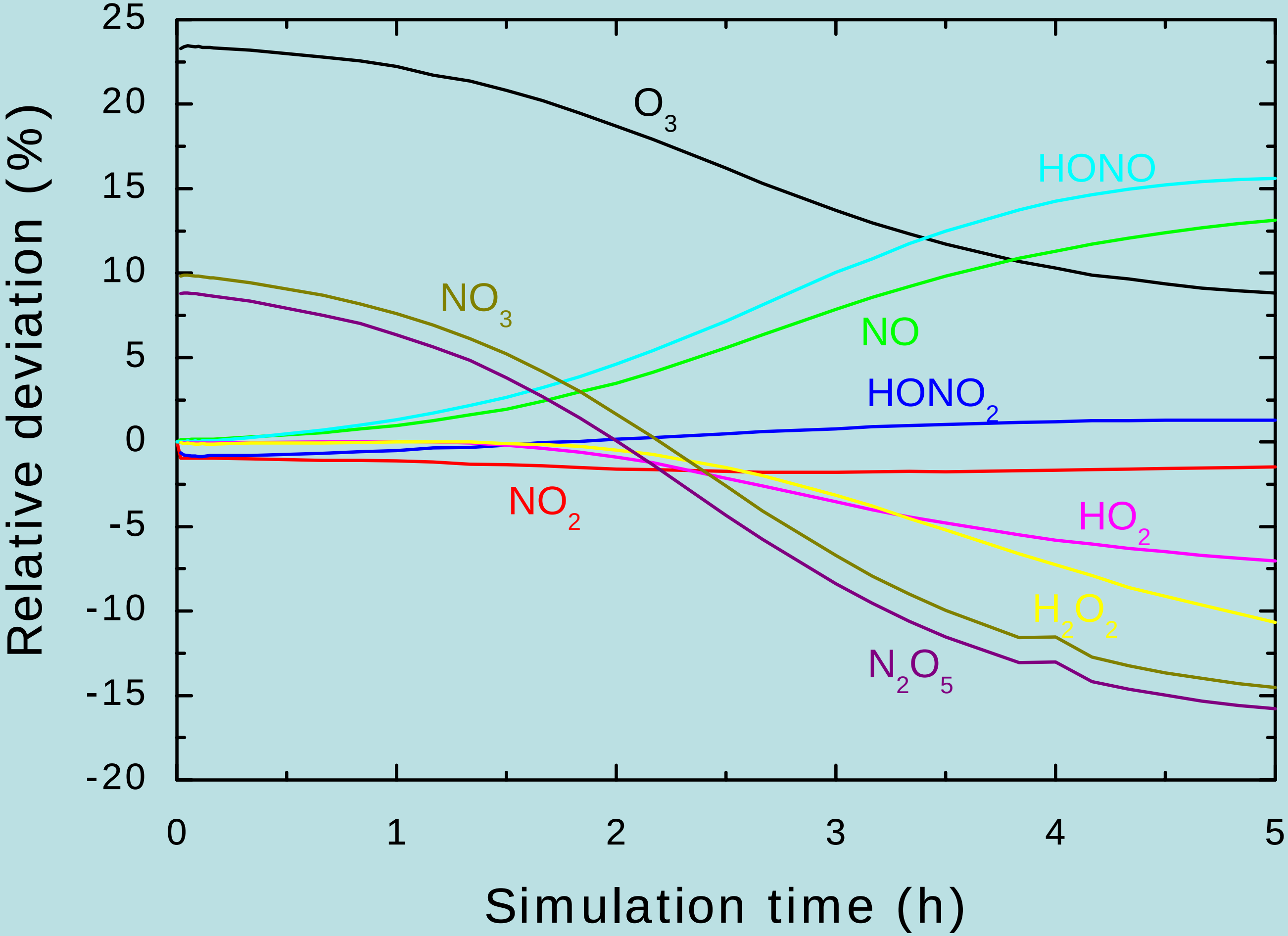
Intensity of segregation



Source: Kramm & Meixner (2000)

Seinfeld-type model for photochemical smog (Kramm, 1987, 1995)

- 27 species and 53 chemical reactions (26 inorganic and 27 organic)



Source: Kramm & Meixner (2000)

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First principle of thermodynamics (balance equation for enthalpy)

$$\bar{\rho}\frac{d\hat{h}}{dt} - \frac{d\bar{p}}{dt} + \nabla\cdot\left(\overline{\mathbf{R}} + \overline{\mathbf{J}_h} + \mathbf{F}_h\right) = \overline{\mathbf{v}''\cdot\nabla p} - \overline{\mathbf{J}} : \nabla\hat{\mathbf{v}} - \overline{\mathbf{J}:\nabla\mathbf{v}''}$$

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \hat{\mathbf{v}}\cdot\nabla \qquad \text{Euler's operator}$$

Assuming local thermodynamic equilibrium leads to

$$c_p\,\bar{\rho}\frac{d\hat{T}}{dt} - \frac{d\bar{p}}{dt} = \boxed{-\nabla\cdot\left(\overline{\mathbf{R}} + \overline{\mathbf{J}_h} + \mathbf{F}_h\right)} + \overline{\mathbf{v}''\cdot\nabla p} - \overline{\mathbf{J}} : \nabla\hat{\mathbf{v}} - \overline{\mathbf{J}:\nabla\mathbf{v}''}$$

$$\boxed{-\sum_{m=0}^{N}\left(\hat{h}_m - \hat{h}_k\right)\overline{\sigma_m}} + \sum_{m=0}^{N}\left(\hat{h}_m - \hat{h}_k\right)\nabla\cdot\left(\overline{\mathbf{J}_m} + \mathbf{F}_m\right)$$

release or consumption of energy when chemical reactions and/or phase transitions occur

Turbulent closure

Usually: Flux-gradient relationship (Boussinesq, 1877)

$$\mathbf{F}_i = -\bar{\rho}\,\mathbf{K}_i \cdot \nabla \hat{\chi}_i$$

inappropriate because there is no possibility, for instance, to predict segregation effects

Instead: Second-order or/and higher-order balance equations

2nd order balance equation for constituents

$$\frac{\partial}{\partial t}\left(\overline{\rho\,\mathbf{v}''\chi_i''}\right) + \nabla \cdot \left(\hat{\mathbf{v}}\,\overline{\rho\,\mathbf{v}''\chi_i''}\right) = -\boxed{\nabla \cdot \left(\overline{\rho\,\mathbf{v}''\mathbf{v}''\chi_i''}\right)} - \overline{\rho\,\mathbf{v}''\mathbf{v}''} \cdot \nabla \hat{\chi}_i$$

$$-\overline{\rho\,\mathbf{v}''\chi_i''} \cdot \nabla \hat{\mathbf{v}} - \overline{\chi_i''\,\nabla \cdot \mathbf{J}} - \overline{\mathbf{v}''\,\nabla \cdot \mathbf{J}_i} - \overline{\chi_i''\,\nabla p} - 2\,\mathbf{\Omega} \times \left(\overline{\rho\,\mathbf{v}''\chi_i''}\right) + \overline{\mathbf{v}''\sigma_i}$$

Source: Kramm & Meixner (2000)

$$\overline{\chi_i'' \nabla p} \cong c_{p,0} \left\{ \left\{ 1 + \sum_{k=1}^{3} \left(\frac{c_{p,k}}{c_{p,0}} - 1 \right) \hat{m}_k \right\} \overline{\rho \, \chi_i'' \Theta''} \right\} \cdot \nabla \overline{\pi}$$

$$+ \hat{\Theta} \left\{ \sum_{k=1}^{3} \left(\frac{c_{p,k}}{c_{p,0}} - 1 \right) \overline{\rho \, \chi_i'' m_k''} \right\} \cdot \nabla \overline{\pi} + \nabla \left\{ \frac{1}{\overline{\overline{\rho}}} \overline{\rho \, \chi_i'' p} \right\}$$

$$- \underbrace{c_{p,0} \; \overline{\pi' \nabla (\rho \, \chi_i'' \Theta_\nu)}}_{\delta\chi}$$

Source: Kramm & Meixner (2000)

$$\overline{\mathbf{v}''\sigma_i} = \sum_{j=1}^{N} \overline{k_{ij}\,\rho\,\mathbf{v}''\chi_j} + \sum_{\substack{m=1\\ n\geq m}}^{N} \overline{C_{imn}\,\rho\,v''\chi_m\,\chi_n}$$

$$\sum_{j=1}^{N} \overline{k_{ij}\,\rho\,\mathbf{v}''\chi_j} \cong \sum_{j=1}^{N} \hat{k}_{ij}\,\overline{\rho\,\mathbf{v}''\chi_j''}$$

$$\sum_{\substack{m=1\\ n\geq m}}^{N} \overline{C_{imn}\,\rho\,v''\chi_m\,\chi_n} \cong \sum_{\substack{m=1\\ n\geq m}}^{N} \hat{C}_{imn}\left(\overline{\rho\,\mathbf{v}''\chi_n''}\,\hat{\chi}_m + \overline{\rho\,\mathbf{v}''\chi_m''}\,\hat{\chi}_n\right)$$

$$\frac{\partial}{\partial t}\left(\overline{\rho\,\chi_i''\beta''}\right) + \nabla\cdot\left(\hat{\mathbf{v}}\,\overline{\rho\,\chi_i''\beta''}\right) = -\nabla\cdot\left(\overline{\rho\,\mathbf{v}''\chi_i''\beta''}\right) - \overline{\rho\,\mathbf{v}''\beta''}\cdot\nabla\hat{\chi}_i$$

$$-\overline{\rho\,\mathbf{v}''\chi_i''}\cdot\nabla\hat{\beta} - \overline{\chi_i''\nabla\cdot\mathbf{J}_\beta} - \overline{\beta''\nabla\cdot\mathbf{J}_i} + \overline{\chi_i''\sigma_\beta} + \overline{\beta''\sigma_i}$$

β stands for χ_j, Θ and m_k

Source: Kramm & Meixner (2000)

2nd order balance equation for momentum

$$\frac{\partial}{\partial t}\left(\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}\right)+\nabla\cdot\left(\hat{\mathbf{v}}\,\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}\right)=-\nabla\cdot\left(\overline{\rho\,\mathbf{v}''\,\mathbf{v}''\,\mathbf{v}''}\right)$$

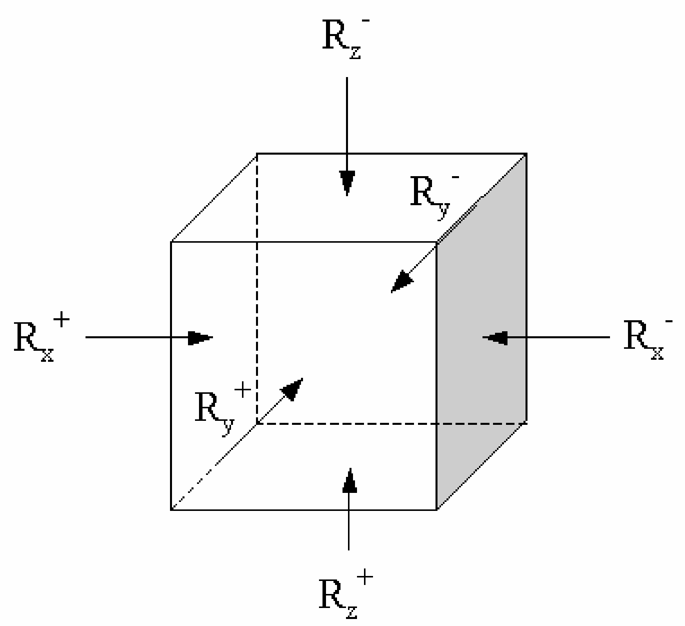
$$-\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}\cdot\nabla\hat{\mathbf{v}}-\left(\nabla\hat{\mathbf{v}}\right)^{T}\cdot\left(\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}\right)$$

$$-\overline{\left(\nabla\cdot\mathbf{J}\right)\mathbf{v}''}-\overline{\mathbf{v}''\left(\nabla\cdot\mathbf{J}\right)}-\overline{\left(\nabla p\right)\mathbf{v}''}-\overline{\mathbf{v}''\,\nabla p}$$

$$-2\,\boldsymbol{\Omega}\times\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}+2\,\overline{\rho\,\mathbf{v}''\,\mathbf{v}''}\times\boldsymbol{\Omega}$$

Source: Kramm & Meixner (2000)

Radiation



Cox (1995)

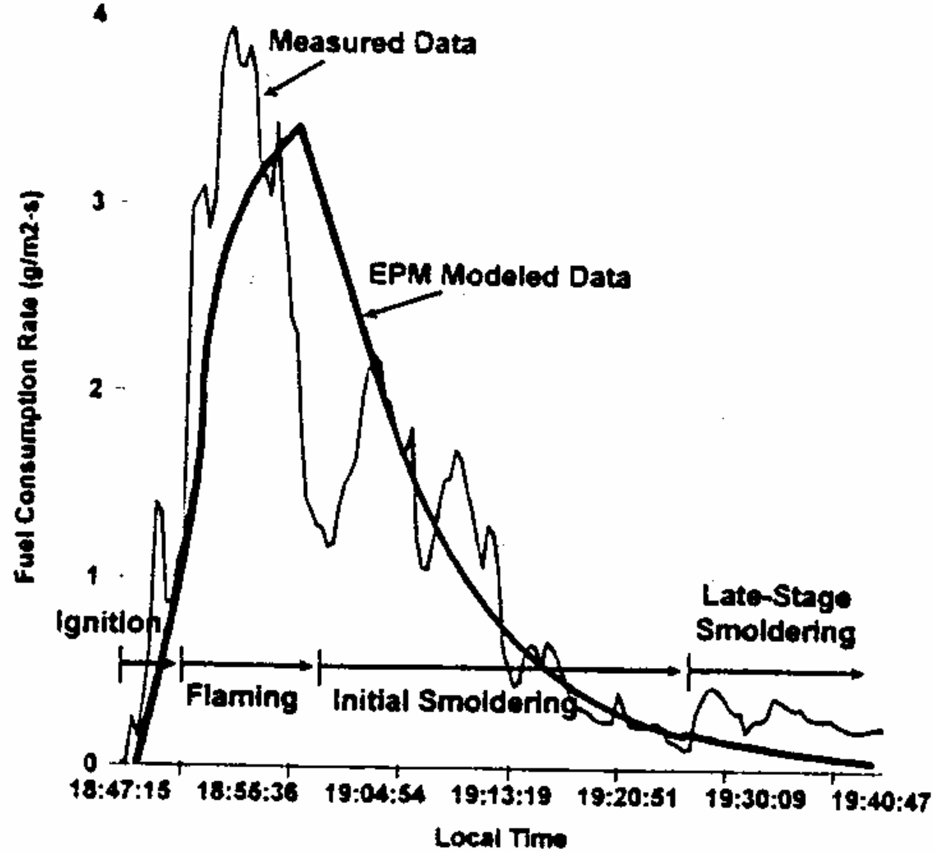
Soil physical processes (effects on permafrost)

HTSVS: Hydro-Thermodynamic Soil Vegetation Scheme, developed by Kramm & Mölders during the last two decades.

It describes the transfer of heat and water within the soil on the basis of the linear thermodynamics of irreversible processes as described by Philip & de Vries (1957) and de Vries (1958), i.e. cross effects like Dufour effect and Ludwig-Soret-effect are allowed. HTSVS also allows freezing and melting of soil water.

HTSVS was evaluated with respect to short-term integration (Kramm, 1987; Kramm et al., 1994, 1996) and long-term integration (Mölders et al. 2003 a,b). It was used in the meso-scale β model GESIMA (Mölders, 1999) and meso-scale α model MM5 (Mölders, 2000; Mölders & Walsh, 2004).

Boundary conditions for flame chemistry



Fuel consumption rate of a typical biomass burn (Ferguson et al., 1998).

Computer performance

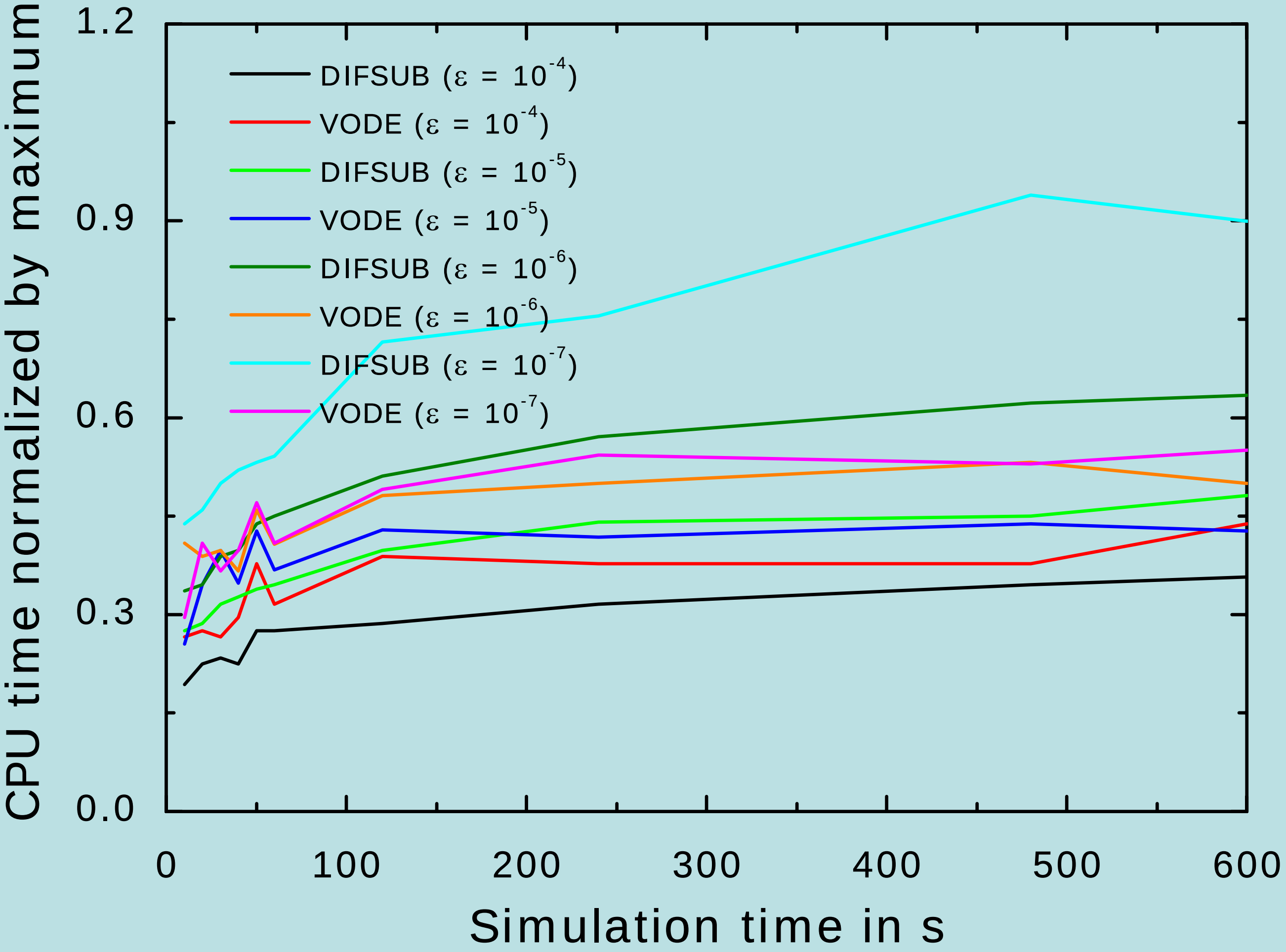
To numerically solve the balance equation of constituents it is indispensable to use an operator splitting technique like that proposed by Russian people Yanenko (1971) and Marchuk (1974) later intensively tested by Seinfeld and collaborators (McRae et al., 1982).

$$\chi^{n+1} = T_x\ T_y\ T_z\ C(2\ \Delta t)\ T_z\ T_y\ T_x\ \chi^{n-1}$$

Advantage: The system of chemical reactions can be expressed by a (stiff) system of ordinary differential equations

Appropriate solvers are: Gear’s (1971) DIFSUB, EPISODE Byrne & Hindmarsh (1975) and VODE of Brown et al. (1989), but these solver always need a huge amount of CPU time.

Results from benchmark tests



Outlook

The requirements on wildfire-atmosphere modeling are:

A meteorological pre-processor like RAMS or a new development that includes

- a set of balance equations for highly reactive species,
- a kinetic mechanism for the flame chemistry by considering segregation effects owing to turbulence,
- a three-dimensional transfer module for thermal radiation,
- a parameterization scheme for the pyrolysis of ground fuel and canopy fuel,
- a parameterization scheme of turbulence that is based, at least, on second-order closure principles to predict eddy flux densities, turbulent diffusion flames and the turbulent dispersion as well as dry deposition of the highly reactive constituents of smoke,
- a kinetic mechanism for simulating photo-chemi-cal processes by considering segregation effects owing to turbulence,

- a multi-layer scheme for tall vegetation with strongly variable leaf area density to realistically predict the transfer and the turbulent mixing of heat, water vapor, and chemical species as well as momentum,
- the thermo-hydrodynamic soil-vegetation model (HTSVS) for predicting the transfer of heat, water vapor, and water within the soil even under permafrost conditions.

Currently, such a wildfire-atmosphere model does not exist.

Model evaluation:

- Observation data from the FROSTFIRE experiment of the NSF Environmental Biology FROSTFIRE program,
- Observation data from the Boundary Fire,
- Observation data from future wildfires.